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A THEORETICAL SEARCH FOR SUPERVELOCITY SEMICONDUCTORS

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EXECUTIVE SUMMARY

This document presents an annual report to the Office of Naval Research for a research program entitled "A Theoretical Search For Supervelocity Semiconductors". This program has been funded by ONR since 1974 in the Department of Electrical and Computer Engineering at N.C. State University. The research has resulted in more than 80 refereed publications and numerous conference presentations from its inception. Major contributions to the field of hot electron transport and semiconductor device modeling have been achieved, new computational methods have been developed (e.g. path integral Monte Carlo techniques), and the work has helped stimulate commercial ventures in the applications of quaternary semiconductor materials to electronic and optical devices. In addition, there have been twenty eight Ph.D. and M.S. students who have received degrees at N.C. State University with research support from this contract. Three visiting faculty members from Japan came to the University to work with the faculty investigators supported under this ONR contract during the 1979-1983 time period. A visiting professor from the French CNRS Microstructures and Microelectronics Laboratory in Bagneux (near Paris) spent a sabbatical year at N.C. State during 1988-89, and he devoted full-time working on this program at no cost to ONR. During the current funding period, a visiting scholar from China is a member of our research group working on projects which directly impact this ONR program. This researcher will be appointed as a Visiting Assistant Professor in August, 1992, and will spend approximately 50% of his time working on this project. His work will be devoted to advanced device simulation and physics. In particular, he will develop new concepts for the real space transfer logic transistor and other charge injection transistor structures. Finally, we have hired a new post-doctoral research associate from the University of Michigan (Prof. J. Singh's group) and he will join us to work on transport theory in various quantum-based devices.

This initial phases of this work centered around the development of Monte Carlo simulation techniques which allow the study of detailed physics of hot electron transport in a variety of compound

semiconductor materials. The original emphases were concerned with electronic materials phenomena. Later work considered the utilization of these materials in realistic device structures where physical boundary conditions must be imposed on the carrier transport. More recently, the work has focused on the domain of ultra-small materials and device phenomena where microscopic non-local transient effects such as velocity overshoot, ballistic and nearly-ballistic transport, and quantum transport become important or dominant. During the past five years we have researched the applications of the Feynman "integral over paths" approach to quantum transport and identified numerical limitations to its practical application. Also we have emphasized the study of hot electron effects in new device structures, such as the hot electron spectrometer, heterojunction bipolar transistor, small dimension metal-semiconductor-metal photodetectors, delta-doped high electron mobility transistors, and real space transfer logic transistors. During this time, we have been exploring some new approaches to device modeling which combine the Monte Carlo method with the method of moments of the Boltzmann transport equation (hydrodynamic transport model) for studying specific device structures, such as small-dimension $n^+\!-\!n\!-\!n^+$ majority carrier devices and the high electron mobility transistor. In addition, we have incorporated quantum correction terms into the hydrodynamic model and applied this model to resonant tunneling structures. Recently, we have applied a new ansatz distribution function as a constitutive relation to close the moment equations in the hydrodynamic transport model. Initial results of this approach have been physically satisfying and computationally promising. A comprehensive formulation of this new model has been published and has attracted a lot of attention.

During the next year, new research in four general areas will advance our basic research directions encompassing the study of hot electron transport in materials and devices. These four areas included 1) the study of quantum transport in mesoscopic structures, nanostructures, and related ultra-small heterobarrier device structures using several physical models and computational approaches, 2) new approaches to the merging of Monte Carlo methods with moment equation methods with resulting improvements to the hydrodynamic transport model, 3) Monte Carlo simulations in order to study

pseudomorphic devices, real space transfer structures, and submicron MOSFETs, and 4) search for new quantum-based device concepts for ultra-fast, ultra-dense applications. The possibility of expanding our experience to optical and optoelectronic device modeling will be seriously explored as well, as we define the role of our new personnel which will be added to our group in Fall 1992.

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1.0 INTRODUCTION

In October, 1974, the Office of Naval Research initiated sponsorship of a basic research program in the Department of Electrical and Computer Engineering at North Carolina State University. The general goal of this research program has been and continues to be the investigation of high-speed carrier transport in III-V compound semiconductors, III-V alloy materials, other advanced electronic and optical materials, and novel device structures which utilize these materials. Four faculty members at N. C. State have been primarily involved and supported by this project. Currently, Profs. M. A. Littlejohn and K. W. Kim serve as the co-principal investigators on this project. This research program has made significant contributions to the understanding and knowledge base of hot electron transport in materials and devices. It has provided scientific guidance to the U. S. Navy in the formulation of a part of its basic and applied research program. Numerical concepts developed under this project have been transferred to other Universities, including the University of Illinois, and we continue these inter-institutional collaborations. During the past year, we have maintained close contact with the research program of Prof. Hess at the University of Illinois. Also, collaborations with Dr. H. L. Grubin of Scientific Research Associates, Inc. and Dr. G. J. Iafrate and Dr. M. A. Stroscio of the U. S. Army Research Office in the area of quantum transport in semiconductor devices have been strengthened. Dr. Iafrate, Dr. Stroscio, and Dr. Grubin are Adjunct Professors in the ECE Department at North Carolina State University and we share graduate students and post-doctoral research associates on joint projects. In addition to those directions, our research results have helped stimulate commercial ventures, particularly in the development of GaInAsP-based materials and devices. To-date, this program has resulted in 79 refereed publications in the literature, 1 additional manuscript is currently in press, and 6 manuscripts have been submitted or are in preparation for submission to the technical literature. A listing of these publications is given in Appendix A. In addition, numerous invited talks and presentations have been given at conferences and workshops throughout the United States and in

other countries. The program has contributed significantly to the educational program at N. C. State University with more than thirty Ph.D., M.S. and undergraduate students having received support under this ONR contract. Currently, three Ph.D. students are working toward their degrees on this project. Two of these Ph.D. students are U.S. Citizens. A visiting scholar from China, who will be appointed as a Visiting Assistant Professor in August, 1992, is also working on research related to this program. We have hired another post-doctoral research associate who will extend our capabilities into the area of band structure effects, quantum transport, and many-body physics.

This ONR program has been efficient and productive. The high quality of this research will continue to be maintained in the future. This report summarizes the progress and accomplishments made during the past contract period.

2.0 RESEARCH RESULTS

2.1 Background

Since its inception, semiconductor technology has been stimulated by requirements for electronic systems with ever-increasing capabilities to process information faster, more functionally and more efficiently. These requirements have motivated the scaling down of integrated circuit (IC) device dimensions into the submicron (less than ten thousand angstroms) and ultrasubmicron (less than one thousand angstroms) regions. Today, we have entered an era where nanostructure physics and fabrication motivate our research efforts in semiconductor electronics [1]. As fabrication technology has allowed such devices to be realized, many new and fundamental questions have emerged concerning the underlying physics of small (atomic level) dimensions in semiconductor devices. Important issues now under consideration for ultrasubmicron devices include nonequilibrium transport dealing with such topics as quasi-ballistic transport, overshoot phenomena and quantum transport. A great deal of progress has been achieved in our understanding of these important device effects, although major work remains to be done as our ability to fabricate very small electronic device structures continues to expand and mature [2,3].

The ability to fabricate small devices has been continually refined over the last ten years through impressive improvements in materials growth technologies. Molecular beam epitaxy (MBE), metalorganic chemical vapor deposition (OMCVD), and atomic layer epitaxy (ALE) have provided the ability to fabricate a wide variety of materials and heterostructure combinations with near perfect interfaces, doping control and compositional uniformity with atomic level dimensions. The development of ALE may very well prove to be the ultimate growth technology since it allows the deposition of one monolayer of device quality materials through a controllable, self-limiting mechanism, and is especially useful for the deposition of heterojunctions [4]. The ability to grow layers with dimensions of a few angstroms opens the domain of quantum transport to experimental study and verification. Thus, topics

resulting from size quantization in condensed matter must be investigated from theoretical viewpoints with tools which are either partially developed or through the development of new tools which are not now available. Quantization effects arising from geometrical size constraints, proximity effects resulting from closely packed arrays of devices, and general solid-state considerations not heretofore considered questionable (effective mass approximation, the role of contacts and the like) must be addressed from a fundamental point of view. Moreover, from a device physics point-of-view, it is desirable to have a microscopic description of the physics of small dimensions which is amenable to phenomenological treatment, so that its properties can be meaningfully incorporated into futuristic device concepts and simulations.

Theoretical methods to address carrier transport have also progressed rapidly over the last ten-fifteen years, in a manner similar to research in semiconductor thin film epitaxial growth technology. In fact, this is a natural progression in many ways and is to be expected. The progress achieved in materials growth of structures with quantum dimensions dictates that new approaches be developed and refined to study quantum transport phenomena and the physics of small dimensions. However, a significant change in direction is now warranted. Past transport theory and device modeling approaches have relied on particle or quasi-particle approaches where the electrons are treated as rigid mobile entities which undergo interactions with the transport medium. The treatment of the interaction often involves wave concepts. However, the model is basically a particle model. In the current regime of quantum transport, we may no longer be able to consider the carriers as particles. It is quite likely that their physical behavior will be governed either partially or completely by wave phenomena.

Quasi-particle methods are an attempt to model structures with quantum dimensions which retain as much of the classical formalism as possible in order to be able to express results in terms of parameters which are of the greatest experimental interest, such as carrier velocity and diffusion constant. This is a flexible approach. However, much care is required to ensure that all important effects are

properly included because of the approximations involved in the formulations. On the other hand, more fundamental quantum approaches, such as operator-eigenfunction methods, adhere closely to the actual quantum states present in the device structure when scattering is not included. Scattering processes (dissipation) can be added by using perturbation theory from quantum mechanics. These techniques can obtain the greatest sensitivity to the resulting carrier confinement and the lattice potentials. However, they are relatively inflexible in studying non-linear dynamical properties in the presence of strong dissipation, such as is present in the electron-phonon interaction at high electric fields.

Another approach to quantum transport relies on the "integral over paths" method, originally proposed by Dirac and formulated by Feynman [5]. Practical path integral methods for the study of small devices rely on an influence functional technique in which the source of the dissipation has been integrated over all phonon modes. This results in a model influence functional where the phonon-scattering dissipation can be represented as an interaction with a collection of harmonic oscillator modes in which the translational invariance of the carriers is preserved. The resulting model includes constant or oscillatory electric and magnetic fields, carrier screening, scattering and dissipation, carrier confinement, background temperature and initial conditions can be dealt with as readily as for a free particle [6]. The path integral method can be compared and contrasted to other methods now being studied and supported by ONR, such as the application of the density matrix formalism and Wigner distribution function approaches including the use of moment equations [7]. Based on our progress in developing the path integral approach during the past five years, we believe that path integral methods will play an important role in developing an understanding of quantum transport in reduced geometries (such as mesoscopic devices [8]). However, because of its intensive computation requirements, the path integral method is very limited in its application to practical devices. Currently, we are aware of only one other U.S. university program directed toward applying the path integral method to semiconductor devices. This is the program at the University of Illinois under the direction of Prof. Karl Hess. Our efforts in the development of this method are complimentary to the one at Illinois, and we have

collaborated with the Illinois personnel through the use of the NSF Supercomputing Center and the National Center for Computational Electronics located there. One of our former students, whose Ph.D. dissertation on path integral methods was supported by this ONR contract, joined Prof Hess' group in January, 1990 as a Visiting Research Assistant Professor. We plan to maintain contact with Prof. Hess' group as we evaluate our path integral research directions. We will continue this work if we can hire an appropriate Ph.D. candidate.

The work at N. C. State University supported by the ONR under the current contract has progressed over the past fifteen years from the realm of particle models to quasi-particle models to quantum transport models. We have relied primarily on the Monte Carlo method to study and solve transport problems in III-V compound semiconductors. Our techniques for modeling materials physics and device phenomena extend to device dimensions around one thousand angstroms [10,11], and we are confident in these models for predicting steady state and transient device effects down to these dimensions. However, in order to remain in the forefront of transport physics and device research, we must continue and increase our progress into the realm of dimensions where physical effects can be studied in device regions with dimensions less than one thousand angstroms. We will continue to explore the Monte Carlo transport method for study of novel device structures where theoretical underpinning is required. One novel class of structures which will be studied in detail by the Monte Carlo method is based on the rapidly-emerging pseudomorphic or strained-layer devices. These structures permit extended compositional ranges and, thus, have a number of potential advantages such as higher transconductance and channel carrier density. Recent studies on the strain-induced piezoelectric fields have opened yet another possibility in realizing ultra-fast switching devices, resulting in an increased importance on the study of carrier transport in these devices. Other novel devices which will be analyzed include delta-doped field-effect transistors and real-space transfer devices, based on studies which have begun during the past two years. In addition, we will incorporate Monte Carlo methods into the quasi-particle approach based on moments of the Boltzmann transport equation with quantum

mechanical corrections. Preliminary results show the utility of this approach for modeling microwave and millimeter wave devices which are important to the DoD's MMIC program.

Finally, we want to re-iterate the important interactions which have developed between our research group and other researchers during the last year. These interactions increase the impact of this program on the field of semiconductor device physics and allow our research efforts to be far more productive through increased intellectual efforts and enhanced facilities and resources. During the 1991-1992 funding period, we have maintained collaborations with Prof. K. Hess at the University of Illinois, Dr. H. Grubin of Scientific Research Associates, and Drs. M. Stroscio and G. Iafrate of the U. S. Army Research Office. These research collaborations have resulted in several joint publications based on mutual research interests, expertise and capabilities. There have been several visits between these laboratories and the logistics for increased collaborations are excellent.

Thus, we believe that we have a well-rounded approach for this ONR program which will lead to new innovations, and practical developments in semiconductor device physics, simulation and modeling.

2.2 Summary of Research Results

This section provides the current status of our research efforts in specific topical areas we have worked during the past year.

2.2.1 Hydrodynamic hot-electron transport model

The primary goal of this research is to develop and implement an advanced hot-electron transport model suitable for accurate and efficient study of electron dynamics in both submicron and ultrasmall semiconductor device structures. The model is required to accurately reflect hot-electron effects such as velocity overshoot and nonstationary effects due to spatial nonuniformities in average electron concentration, average electron velocity and average electron energy. Also, the model is required to accu-

rately describe the streaming motion and dissipation of electrons in multiple nonparabolic conduction bands (as are present in especially all III-V compound semiconductors). In addition, an electron transport model is desired which can be extended to the study of quantum systems (i.c., feature sizes less than 1000 Å) where wave-like characteristics (e.g., tunneling and interference effects) are important.

Over the past decade, much effort has been focused on the development of semi-classical electron transport models which accurately reflect hot-electron effects in submicron semiconducting device structures [11]. The incentive is that nonequilibrium and/or nonstationary effects may be employed to achieve superior electron device performance. One important example of a potentially useful hot-electron effect is velocity overshoot [12]. In velocity overshoot, the difference in momentum and energy relaxation times can result in an initial temporal drift velocity, under constant electric field conditions, which overshoots the corresponding time steady-state (stationary) value. This dynamical response in electron motion is due to the difference between the displacement of the electron distribution in momentum space and the displacement in energy space (i.e., the form of the nonequilibrium distribution function). For this type of electron motion, one cannot use simple models based upon stationary relationships (which ignore important features of the distribution) to describe the transport physics. Furthermore, deficiencies in these near-equilibrium models may also fail to accurately describe electron transport in submicron device structures even in time steady-state. This can occur when the electron gas is far from equilibrium and large spatial gradients in the electron gas parameters (electron density, average electron velocity, average electron energy, etc.) exist.

Since classical (drift-diffusion) models assume local stationary relationships (average velocity depends on the local electric field) and are based upon near equilibrium derivations [12], physically superior models must be used to fully and effectively study important hot-electron effects. At present, the problem of treating transport in submicron structures is typically attacked using one of two distinct methods. The first and most accurate approach has been to apply Monte Carlo simulation methods

[13]. The Monte Carlo method is a powerful statistics-based numerical technique for investigating electron transport physics in semiconductors and semiconductor devices [13]. While the Monte Carlo method provides a relatively simple and accurate indirect approach to determine particle distribution functions and transport parameters resulting from the Boltzmann transport equation subject to complex scattering mechanisms, the approach does have important disadvantages. Specifically, the technique often requires extensive computation time to arrive at adequate statistics and does not naturally possess macroscopic terms for physical interpretation.

The alternative (second) approach to study electron device physics more accurately and efficiently is to develop macroscopic models which predict average transport quantities as opposed to the full electron distribution function. In this approach, the description of electron dynamics is reduced to hydrodynamic-like conservation equations for electron density, average electron momentum, average electron energy, etc [14]. The hydrodynamic models are derived from moments of the Boltzmann transport equation which usually include many simplifying assumptions (i.e., usually neglect conduction band nonparabolicity, treat multiple conduction band valley effects indirectly and directly or indirectly make incorrect assumptions about the form of the electron distribution function) about the electron transport physics. However, if advanced hydrodynamic models, which include hot electron effects such as multiple nonparabolic conduction bands, are developed and combined with Monte Carlo techniques this is an excellent overall approach. A limited number of Monte Carlo simulations can then be utilized to verify the accuracy of the simplified models and to supply approximate parametric dissipation data for the particular materials and/or devices under consideration. These types of advanced hydrodynamic models, together with the Monte Carlo method, represent a simplified mathematical approach for accurate and efficient study of realistic transport physics.

Finally, very few hydrodynamic (macroscopic or average ensemble-electron) models have been implemented to accurately represent quantum effects (i.e., tunneling and interference) present in

ultrasmall electron structures. One method to accurately model structures with spatial dimensions on the scale of the de Broglie wavelength (i.e., in the quantum regime) is to utilize quantum hydrodynamics [15,16]. In this method, a set of quantum moment equations are derived by taking moments [17] of the Wigner-Boltzmann equation and closure is obtained using an approximate nonequilibrium form of the zero-current (equilibrium) Wigner distribution function. This procedure results in a set of quantum-corrected hydrodynamic transport equations which have been demonstrated to predict quantum phenomena [15,16].

During the past year, advanced forms of the hydrodynamic transport model (HTM) were developed and utilized to study both submicron and ultrasmall semiconducting device structures. First an advanced semi-classical hydrodynamic transport model was developed and implemented to accurately predict electron dynamics in multiple nonparabolic energy bands. In addition, a new quantum mechanical formulation of the first three moment equations (i.e., quantum hydrodynamic equations for electron density, average velocity and average energy) was investigated and implemented to predict non-classical tunneling in a double-barrier heterostructure. The development of the advanced model(s) was achieved through several separate theoretical investigations.

First, to determine a method to include the effects of conduction band nonparabolicity into the macroscopic streaming (collision independent) of the semi-classical HTM, the fundamental physics of electron transport were investigated. An alternate formalism was developed for deriving a new nonparabolic hydrodynamic transport model adequate for modeling hot electron transport in submicron semiconductor devices. Specifically, the model equations were developed by applying a unique set of moment operators ($\Phi_0(k)=1$; a constant, $\Phi_1(k)=u(k)$; the nonparabolic velocity, $\Phi_2(k)=[m(k)/2]u(k)\cdot u(k)=E(k)$; an approximation to the particle energy) to the collisionless Boltzmann transport equation. The operators, used in this analysis, represent a significant improvement in the development of the hydrodynamic transport model since they lead to a more compact mathematical

form. This resulting form can be manipulated more easily and reveals clearly the allowable simplifying approximations. An intuition-based distribution function was proposed as a constitutive (essential) relation to close the moment equations. This ansatz nonparabolic distribution function, which is derived in velocity space for mathematical convenience and approximates some of the characteristics of the true nonparabolic distribution function, was then analyzed and used to develop a set of transport parameters. After development, the results from two independent Monte Carlo transport models were used to evaluate the nonparabolic transport parameters. These models were used to investigate electron transport in both stationary (uniform electric field) and nonstationary (ballistic diode) environments. The results of these studies show that there is excellent agreement between this new nonparabolic transport model and the Monte Carlo calculations. Hence, this new nonparabolic transport model presents a viable alternative to studying realistic electronic device structures operating under high bias conditions.

In the previous analysis, specific macroscopic collision terms are omitted. This is done to permit a concise focus on the streaming (collision independent) terms that evolve from the application of nonparabolic conduction bands. The collision terms, which are almost always treated phenomenologically, has been developed separately for a nonparabolic multi-valley system (GaAs). Specifically, multi-valley dissipation is included in the model using an ensemble relaxation time approximation. The numerous intravalley and intervalley relaxation times were calculated using the Monte Carlo Method.

In order to extend the modeling approach to the quantum device regime, a technique was investigated to develop quantum corrections for the hydrodynamic equations. The set of quantum-corrected transport equations which we have developed and investigated were based upon quantum moment equations of Grubin and Kreskovsky [15]. Grubin and Kreskovsky previously constructed a set of quantum balance (hydrodynamic) equations applicable for electron transport in mesoscopic structures. Their model was derived from the general moment equations of Stroscio [17] using the displaced none-

quilibrium Wigner distribution function of Ancona and Iafrate [18]. These resulting quantum hydrodynamic equations incorporate quantum effects through the introduction of terms (corrections) with density gradient dependence.

Both the advanced semi-classical and the quantum-corrected hydrodynamic transport models (HTMs) were used to study electron transport in novel semiconductor device structures. A general numerical algorithm was implemented to solve the resulting system of nonlinear differential equations [from both physical model(s)] for arbitrary one-space-dimensional n-type structures. The numerical algorithm utilizes a local simultaneous-coupled (Newton) iteration approach in tandem with a global physics-based continuation. Simulation results were generated for a single-valley (Γ) HTM, with quantum corrections, applied to a double-barrier heterostructure with $Al_xGa_{1-x}As$ barriers. This study was the first to use the *three* quantum hydrodynamic (QHD) equations to study transport in heterostructure devices. The key additional feature of the QHD equations is the incorporation of the effects of density gradients through the quantum potential. Insofar as a classical solution does not exist in the presence of barriers, Q (i.e., one of the major quantum correction terms) must at least partially cancel the effects of the barriers and permit carrier transport. Indeed, as is shown in Fig. 1, $Q/3$ does approximately balance the barrier potential which is a result consistent with Ref. 15. In this work, the quantum corrected HTM was used to demonstrate that the hydrodynamic approach can be used to study ultrasmall electron devices.

In another simulation study, a simplified form of the multi-valley hydrodynamic transport model was used to investigate the feasibility of utilizing the velocity overshoot effect in reducing electron transit time through submicron GaAs electronic device structures. In this initial investigation with the new *multi-valley* model, which incorporates a separate set of hydrodynamic equations for each conduction band (Γ, L, and X) and allows for electron exchange through energy dependent relaxation parameters, the nonparabolic correction terms were be suppressed. This was done to simplify the analysis and
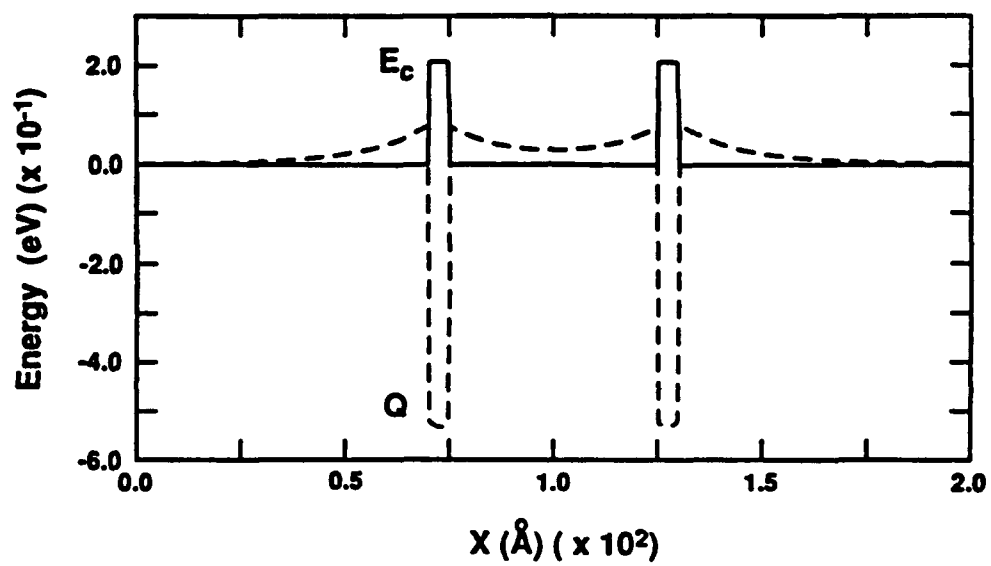
Figure 1: Conduction band (E_c) and quantum potential (Q) at $\mathcal{V}_{applied} = 8mV$. The source and collector regions are excluded from the plot.

to provide a base for future nonparabolic studies. This new multi-valley model was applied to a novel submicron GaAs ballistic diode structure with bandgap engineered electric field spikes (and/or doping spikes) in order to reduce upper valley occupancy and enhance device transit time using the velocity overshoot effect. The general results of the study (summarized in Fig. 2) indicate that, while velocity speed-up is minimal in the neighborhood of the active (low-doped or high-electric field) region, velocity overshoot can be extended into the collector (low-electric field) region with significant transit time enhancement. Since these results are consistent with other independent investigations using more accurate (Monte Carlo) techniques, this work has proven that HTMs are a viable alternative to these more computationally intensive methods.

We have also determined the impact of k-space transfer (i.e., intervalley transfer) and band nonparabolicity on electron were determined. In this work, variations of the multi-valley (Γ, L, and X) nonparabolic hydrodynamic transport model was used to study a submicron GaAs ballistic diode. Numerical simulations indicate that accurately including the effects of nonparabolicity in the streaming terms and k-space transfer in the velocity and energy equations is very important in correctly determining the conductance of the device. The existence and amount of negative differential conductance was determined to be strongly influenced by both of these physical factors. Furthermore, the sensitivity of device conductance to changes in the thermal conductivity is diminished significantly when nonparabolicity is accurately incorporated. Results for the total current density versus applied bias, for different variations in the model are given in Fig. 3. These simulations have demonstrated the pronounced effects of conduction band nonparabolicity and k-space transfer on electron transport in a GaAs ballistic diode. Therefore, the study of nonequilibrium and nonstationary electron physics should be performed with this type of advanced macroscopic transport model.

More recently, work has been performed to develop an *extended* Scharfetter-Gummel current-density discretization formula sufficient for solving an advanced hydrodynamic electron transport model
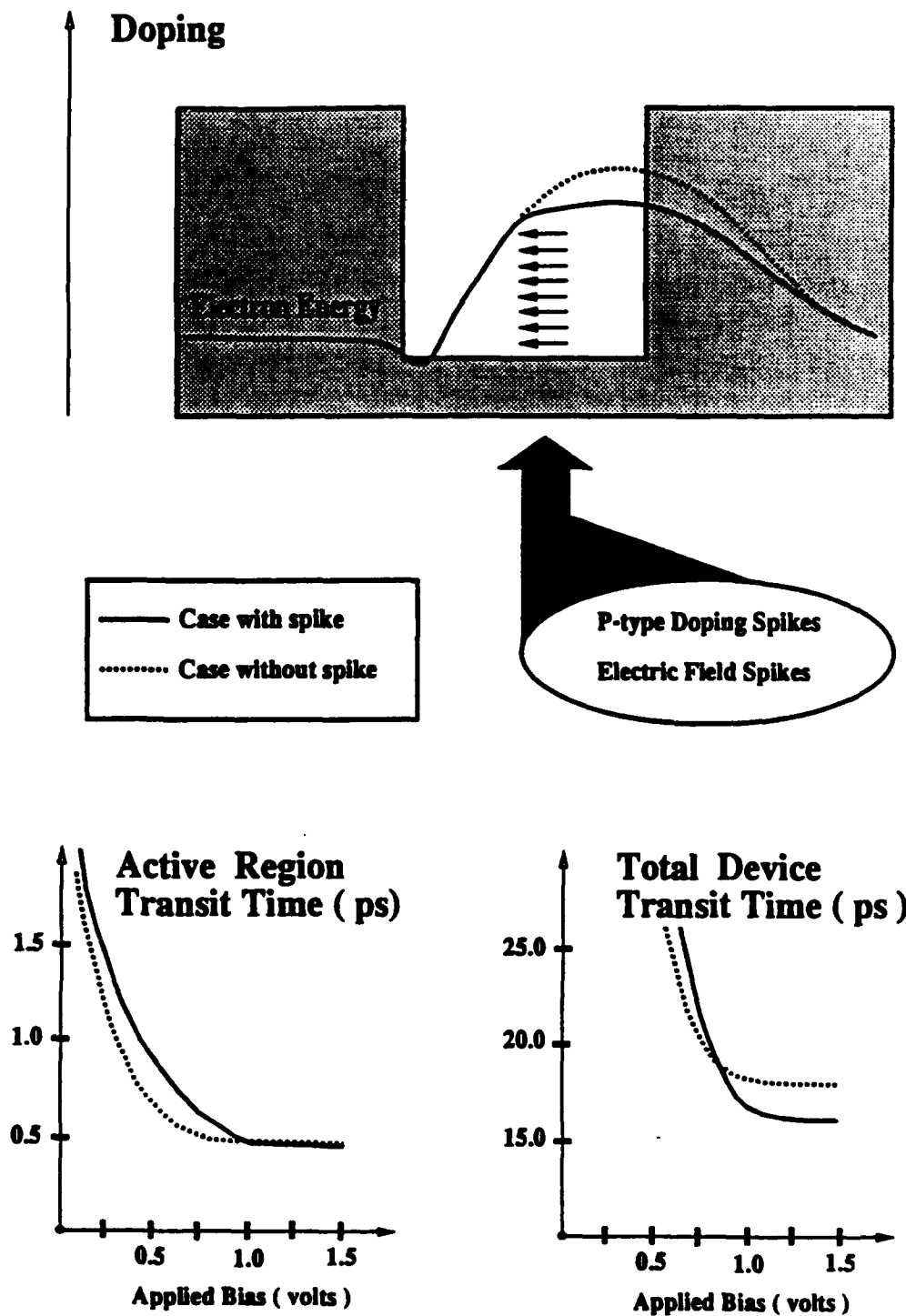
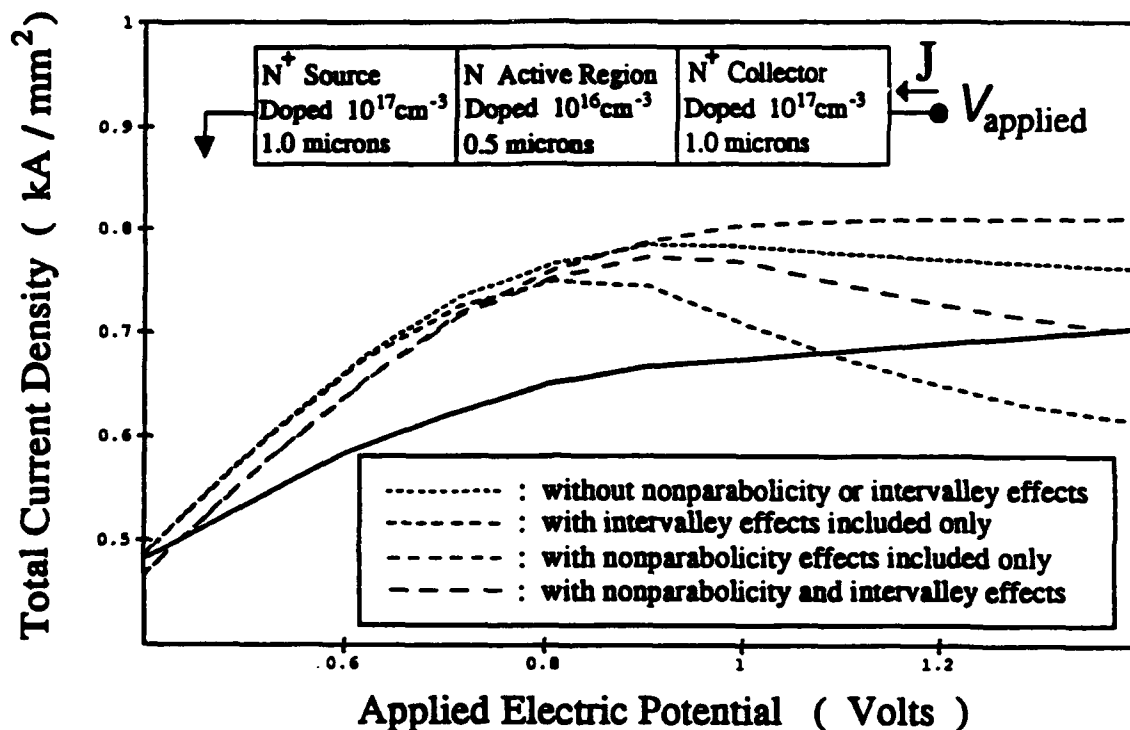Figure 2: Outline of transport study and transit time results

Figure 3: Total electron current density versus applied electric potential for a submicron ballistic diode (BD :see inset). Results are for variations in the hydrodynamic transport model (HTM ; dashed lines) and a Monte Carlo study (MC ; solid line). Four different variations (cases) in the HTM were consider. The results for these different cases are designated by dashed lines with *dash lengths* that increase in the following order. Case A : HTM without nonparabolicity (in the streaming terms) or *full* intervalley effects (in the velocity or energy equation). Case B : HTM with intervalley effects included only. Case C : HTM with nonparabolicity effects included only. Case D : HTM with nonparabolicity and intervalley effects.

(HTM). While this extended formulation properly incorporates many advanced effects associated with hot-electron transport, its primary feature is the accurate treatment of the convection term (or displacement energy term) which is present in both conventional (i.e., drifted Maxwellian model) and the advanced nonparabolic model previously discussed in this report. In general, since the success of any numerical simulation (for a wide variety of device structures and operating conditions) is critically dependent on convergence rate and numerical stability, the choice of an efficient discretization scheme is very important. Currently, most robust discretization formulations for HTMs utilize extensions of the Scharfetter-Gummel (SG) scheme which was found to be stable in drift-diffusion (DD) model simulations. However, most extensions of the SG formula for HTMs either ignore convention terms or else assume *a priori* that they are defined in a previous step of an iteration procedure. A simple analytical approach for directly including convection effects into an extended SG formulation has been established and several versions of this discretization are under investigation. Presently, the stability and efficiency of this new discretization formulation is still under investigation.

Finally, work has been performed to interrogate the influence of different device structures and boundary conditions on the resultant heat flow vector (a transport parameter in the HTM) using the Monte Carlo Approach. Thus far, we have observed that the sign of the heat flow vector is a function of position in ballistic diode structures and that boundary conditions do influence the effective convergence rate (i.e., simulation time to achieve correct symmetry of the electron distribution) of the Monte Carlo method.

2.2.2 Modeling and characterization of novel high speed devices

During the past contract period, we have studied electron transport properties and electrical characteristics for a number of high speed device structures, including delta-doped GaAs MESFETs, AlInAs/GaInAs/InP HEMTs with different additional channel doping characteristics, novel real-space transfer logic transistor structures, and devices with variable doping profiles. The motivations of our

research on these structures are to provide in-depth understanding of electron transport in devices, to investigate the possibility of realizing novel high speed functional device structures, and to provide general design guidelines for optimal device operation.

As a promising high speed device, the delta-doped GaAs MESFET features high current drive capability, high transconductance, improved threshold voltage control, and improved breakdown characteristics. The study of properties of delta-doping in GaAs predicts that device performance of delta-doped GaAs MESFETs is comparable or even better than those of AlGaAs/GaAs HEMTs [19]. However, experimental results show a wide diversity and fall short of theoretical predictions. The design and optimization of device structure (especially delta-doping profile) play an important role in guiding the improvement of device performance. Another high speed device, the AlInAs/GaInAs/InP-based HEMT, has been the focus of extensive experimental study due to superior electron transport properties in this lattice-matched material system. While promising dc and microwave performances have also been achieved, high output conductance has been repeatedly observed for devices with channel-length in the deep-submicron (less than 0.3 μm) regime [20,21]. Physics insight leading to the high output conductance and potential solutions merit careful investigation if potential advantages of AlInAs/GaInAs HEMTs are to be fully exploited. The third device structure which we have investigated this year belongs to a new class of devices which employs the concept of electron real-space transfer [22] in heterojunction structures. The charge injection transistor (CHINT) [23] and the recently-developed CHINT logic element [24] are representative devices. Theoretical predictions and experimental evidence from CHINT operation indicate the possibility for developing novel and improved multi-terminal real-space transfer devices which can realize multiple logic functions. Our last work in the area of device modeling deals with the effects of electron transport in devices with variable doping distributions. Such device structures can be realized by utilizing advanced fabrication techniques, such as focused ion beams or epitaxy (MBE, MOCVD, ALE) methods. The potential advantages of variable doping in device channel or active transport region can best be realized when

detailed electron transport properties in practical device structures are understood and doping scheme optimization is achieved. In the following, we outline the main results of our theoretical study. More detailed descriptions for each subject can be found in the related papers and presentations.

A. Delta-doped GaAs MESFET

Figure 4 gives a schematic illustration of the device structure which we have simulated, along with the delta-doping profile. In this work, we use a two-dimensional, drift-diffusion model to examine the influence of key design parameters on device operation. These parameters are (Fig. 4) peak doping density, half width at half maximum of the doping profile, and distance from the location of peak-doping to the device surface, top layer background doping, and lateral feature sizes. The general design considerations and trade-offs are studied. In particular, our simulation results reveal that: 1) A steeper doping profile and a short gate-to-channel distance are preferred for improvement in device performance. 2) The peak delta-doping concentration and half-width at half maximum of delta-doping profile are found to have a more profound effect than does delta-doping depth (d_p) in enhanced overall device performance. And 3) careful trade-off should be made in the design of top-layer background doping in terms of current drive, transconductance, and threshold voltage sensitivity control. Our results show that a relatively high top layer background doping is preferred to increase drive current and reduce relative threshold voltage shift (due to processing parameter fluctuations) at a cost of a modest reduction in transconductance. Simulation results are in close agreement with measurements from experimental devices fabricated at Texas Instruments using atomic layer epitaxy material prepared in NCSU.

B. AlInAs/GaInAs HEMT

Figure 5 shows the simulated quarter-micron-gate AlInAs/GaInAs HEMT structure which employs different additional channel doping (n^+, i, and p) configurations. The motivation is to study
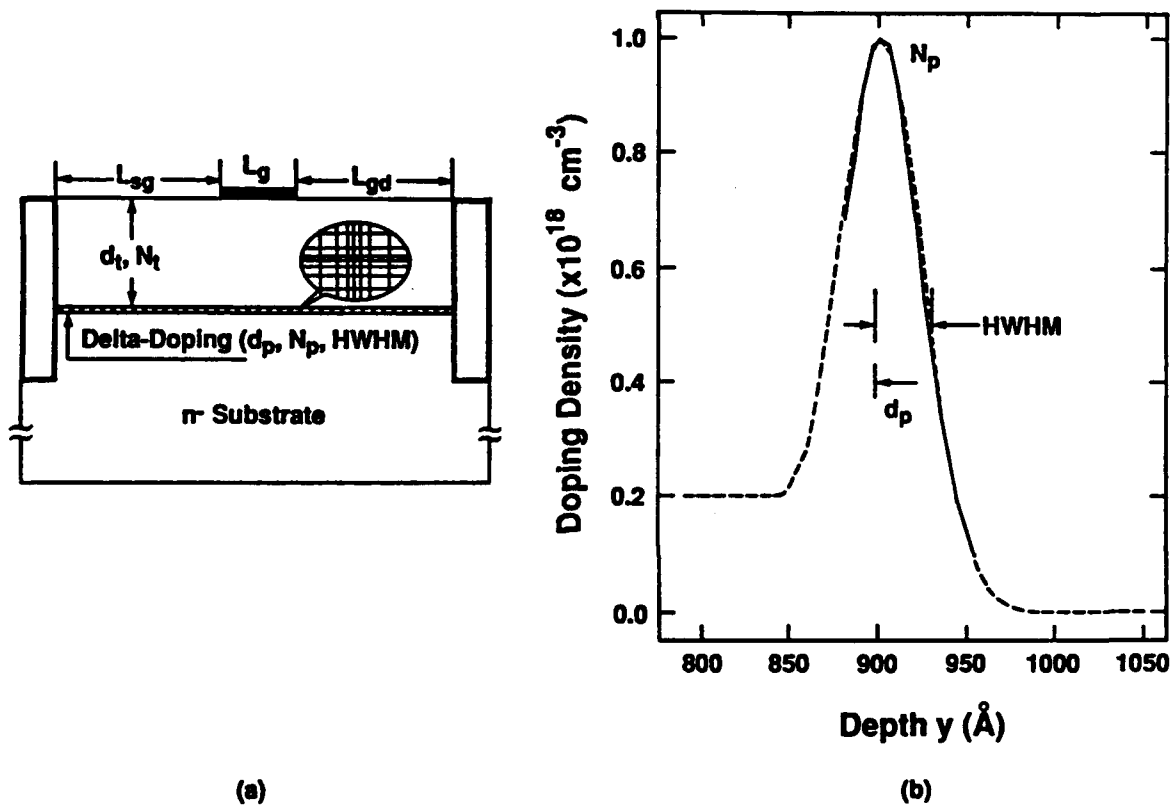
Figure 4: (a) Schematic illustration of a delta-doped GaAs MESFET. The mesh distribution is illustrated in the inset. b) Delta-doping profile. The solid line shows the measurement data and the dashed line shows the Gaussian distribution used in the simulations.

AlInAs-GaInAs HEMTs

GaInAs Contact Layer	7 nm

Undoped AlInAs Layer   20 nm

Donor Layer
(6E18/cm3:12 nm)

GaInAs Channel Undoped or doped @   n(1E17/cm3)
p(1e17 or 3E17/ cm3)

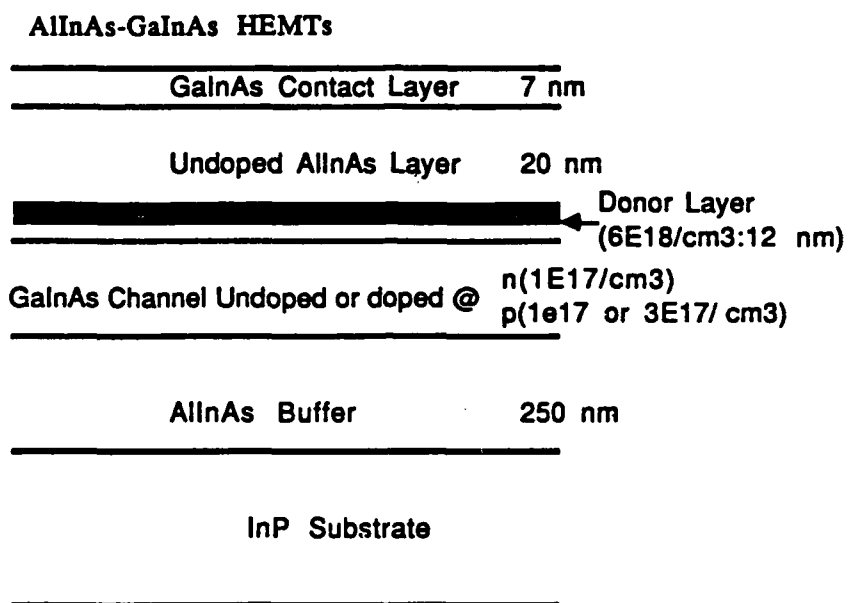AlInAs Buffer   250 nm

InP Substrate

Figure 5: Schematic drawing of the layer structures for AlInAs/GaInAs HEMTs used in this study.

the effect of additional channel doping on device transconductance, output conductance, and high frequency performance. The AlInAs/GaInAs/InP material system appears to be the most promising candidate for high frequency applications. However, for this material system, high output conductance has been an major problem that degrades high frequency performance when the HEMT device feature size is reduced to the ultrasubmicron (less than 0.3 μm) regime. This has been reported by several research groups. Attempts have been made experimentally to reduce output conductance, however, physical insight remains an unknown. In this work, we investigated the possible mechanisms which lead to enhanced or degraded device performance in different char el-doped structures using two-dimensional, self-consistent ensemble Monte Carlo simulations. Our results indicate that conduction in the AlInAs buffer layer and reduced electric field shielding in n-channel doped HEMT are the possible reasons for increased output conductance. By use of a properly designed p-doped channel layer, we observe significantly reduced output conductance and increased trans. Juctance compared with those of n-channel doped HEM l. Detailed analysis indicates that improved electron confinement in the device channel and increase eld shieding for HEMT with p-channel doping improve overall device performance. Our simula as are in reasonable agreement with measurement results from experimentally fabr ated devices [with different additional channel doping (UCSB and Hughes Research Lab)].

C. Real-space transfer logic transistor

The basic real-space transfer logic transistor (RSTLT) is a four-terminal device, which has two separate collectors (C1 and C2) as output terminals when connected through load resistors (R_{C1} and R_{C2}) to the collector supply voltage (V_C); a drain input terminal (D); and a common source terminal (S) which is at ground potential (Fig. 6). The operational principle of the proposed RSTLT is based on the localized nature of real-space transfer of hot electrons in such structures. Channel electrons gain energy from the lateral electric field and real-space transfer occurs when the energy of electrons is comparable to or higher than the heterointerface barrier height. The transferred electrons will be col-
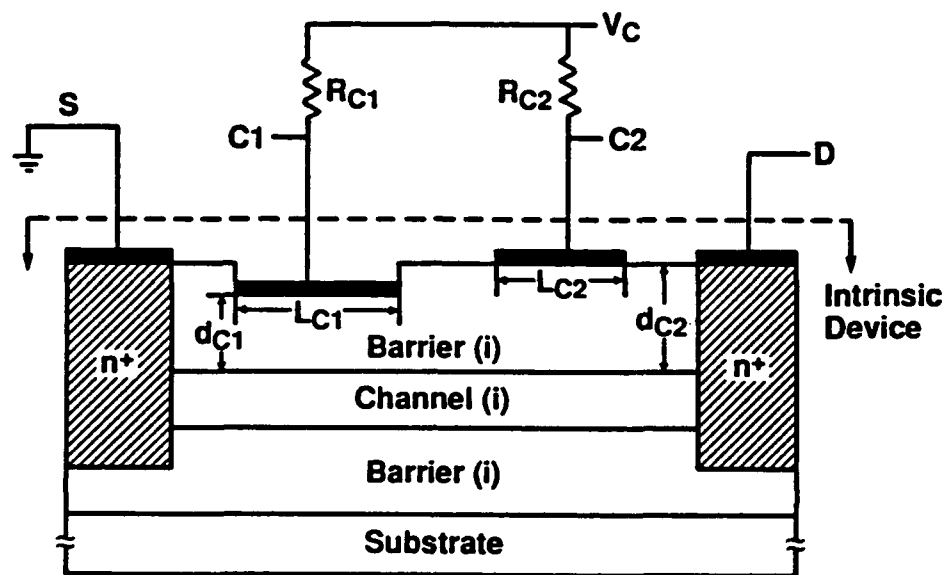
Figure 6: Proposed real-space transfer logic transistor (RSTLT) structure.

lected by either C1 or C2 through vertical electric field. For a given heterointerface barrier height, the spatial location of electron RST is determined primarily by the bias conditions. By properly designing the device configuration and selecting the operating voltages, ultra-fast current exchange between two collectors can be controlled by the applied drain voltage. Compared with CHINT structure, the proposed RSTLT employs: 1) a recessed C1 collector to enhance the vertical electric field intensity under C1 for matched output collector currents, 2) unintentionally doped channel and barrier layers for reduced collector-source and collector-drain leakage currents, and 3) a collector-up device configuration to reduce parasitic capacitance and to facilitate proper arrangement of the device terminals.

In this project, we employ a self-consistent ensemble Monte Carlo model to perform the device feasibility study. Figures 7 and 8 show the current-voltage characteristics and transient current response as a function of time, respectively. A characteristic delay time of about 3.0 psec can be achieved, which would make the RSTLT one of the fastest switching devices reported to date. This characteristic current switching (between two collector terminals) can be utilized to realize a multi-logic element in a single device structure. We have performed case studies to demonstrate that by properly selecting device dimensions and the resistor load elements, collector terminals C1 and C2 can function as logic *NOT* and *EQUIVALENT* of input terminal D. Based on these results, we propose a RSTLT logic element (Fig. 9), which features *NOR/AND* functions (C1 functions as *NOR* of D1 and D2; C2 functions as *AND* of D1 and D2, respectively) and a comparable characteristic delay time as that of the basic RSTLT.

D. Effects of doping variation on electron transport

High performance electronic systems require devices with high current drive capability, high transconductance, high breakdown voltage, and low parasitic resistance. Currently, most semiconductor devices employ doping techniques that control doping profiles in the vertical dimension (e.g., uniform doping, modulation doping, and delta-doping), that is, perpendicular to the direction of carrier
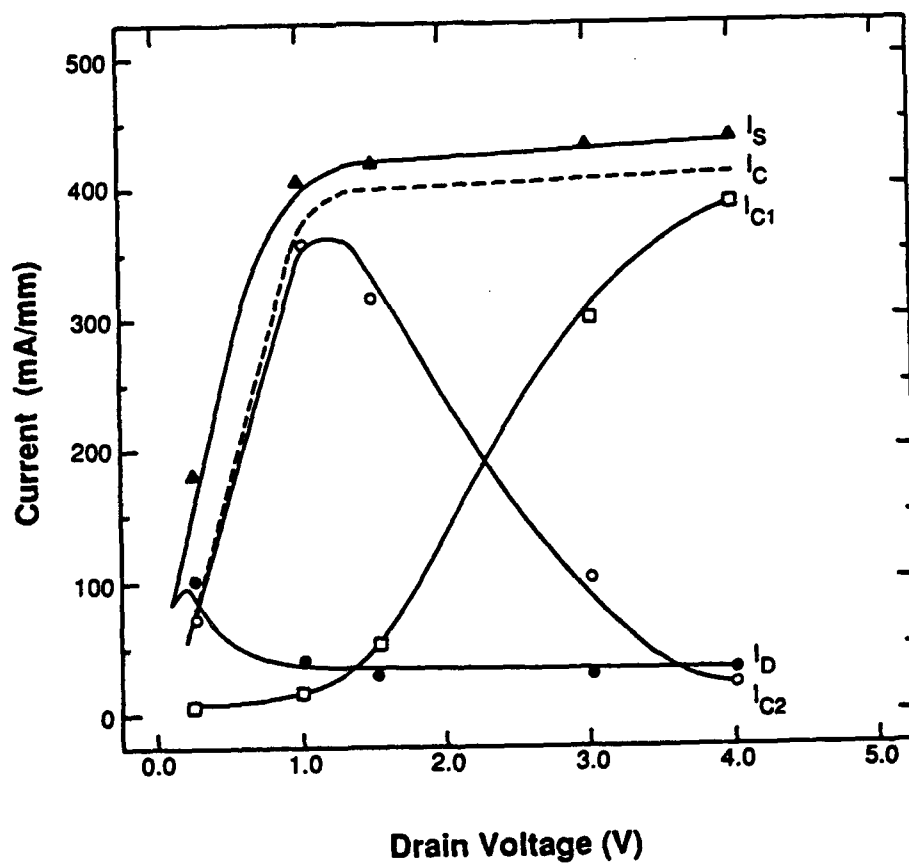
Figure 7: Terminal currents as a function of drain voltage for the $Al_{0.3}Ga_{0.7}As/GaAs$ RSTLT. The collector voltages are fixed at $V_{C1}=V_{C2}=4.0$ V. The dashed line is the total collector current (I_{C1} + I_{C2}).
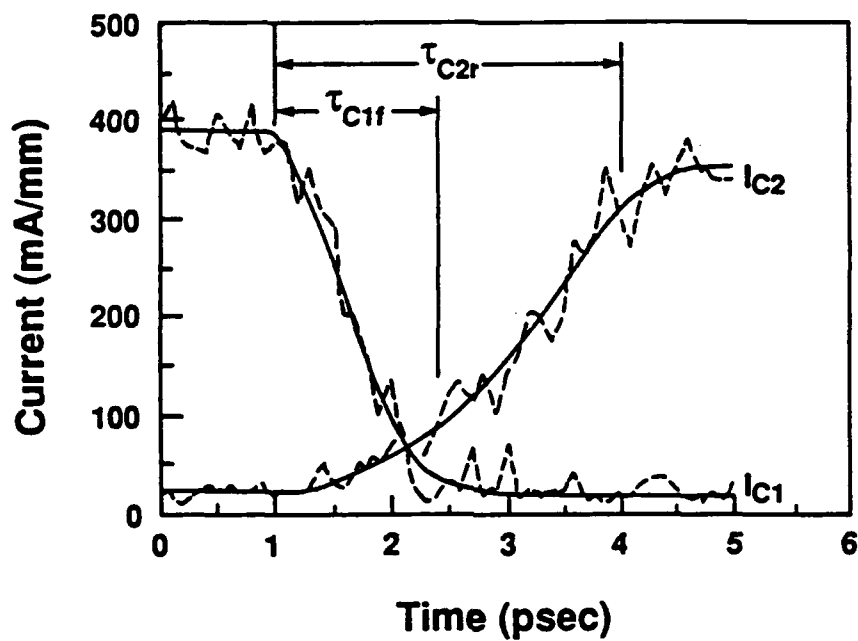
Figure 8: Current response for drain voltage switch-off for an $Al_{0.3}Ga_{0.7}As/GaAs$ RSTLT. The collector voltages are fixed at $V_{C1}=V_{C2}=4.0$ V. The device input (V_D) is switched from 4 V to 1 V at t=1.0 psec.
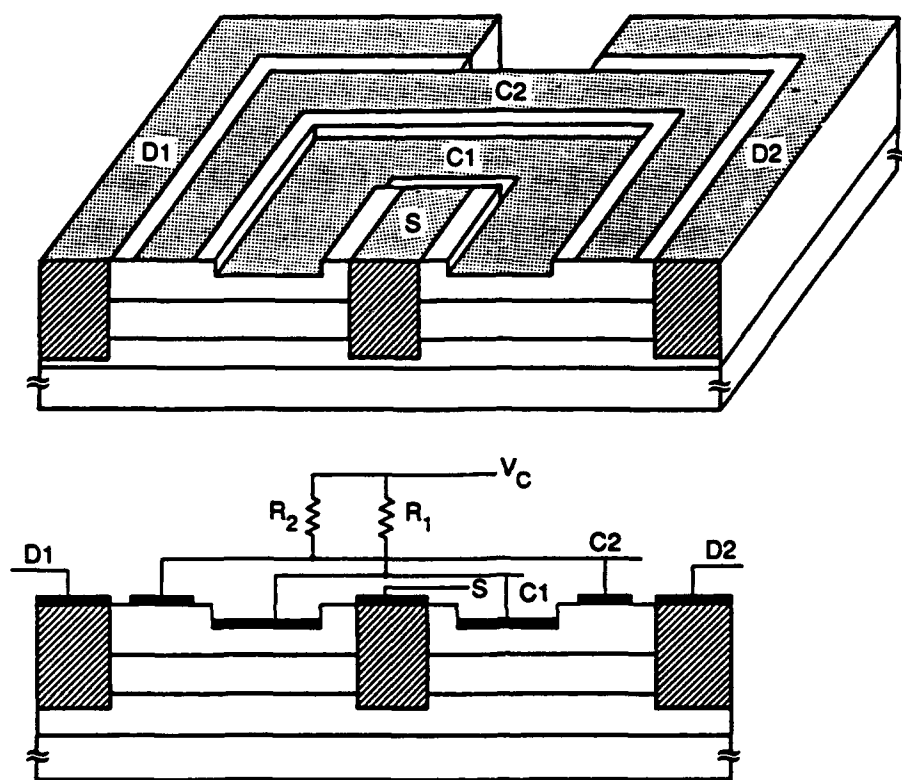
Figure 9: Schematic cross section of a RSTLT *NOR/AND* logic element. The layer arrangement is the same as that in the basic RSTLT structure shown in Fig. 6.

transport. The rapid development of new technologies makes possible changes in doping profile in both lateral and vertical (parallel and normal to carrier transport, respectively). This added degree of freedom for "doping engineering" can possibly result in novel and improved device structures. The motivations of this project are to study the effects of unique variable doping profiles on electron transport properties and to assess potential device applications.

We apply self-consistent ensemble Monte Carlo model to study a GaAs n^+–n–n^+ test device. Doping schemes are ramp-doping (ramp-up and ramp-down) and spike-doping (single-spike and multi-spike) in the n region. In order to have meaningful comparisons among these structures, we apply conditions of identical minimum doping density and the same total integrated dopant in the active n region. Figure 10 shows the current-voltage characteristics of ramp-up (from the left n^+–n junction), ramp-down, and two constant doped structures. Figure 11 compares the current-voltage characteristics for one-spike and three-spike doped structures. It is found for conditions of identical minimum doping density and total integrated dopant in the n region that: 1) the most significant improvement can be achieved by employing a structure with a ramp-down doping scheme. 2) Introducing n^+ spike(s) in the active electron transport (n) region brings improved device performance compared to devices without n^+ spikes. For the one-spike doped structure, electron transport is independent on the location of the n^+ spike. However, less significant improvement is observed for this structure due to the presence of retarding fields over a large portion of the n region. 3) Further improvement can be achieved by splitting one n^+ spike into several spikes in the n region. The redistribution of electron density and the reduced effect of retarding electric fields bring an increased average electron velocity and a resulting higher current drive capability. These results indicate the possibility of enhanced device performances for FET devices which employ proper variable doping schemes. Potential advantages of variable doping in normally-on FET device applications include enhanced current drive, reduced source resistance, and improved breakdown characteristics.
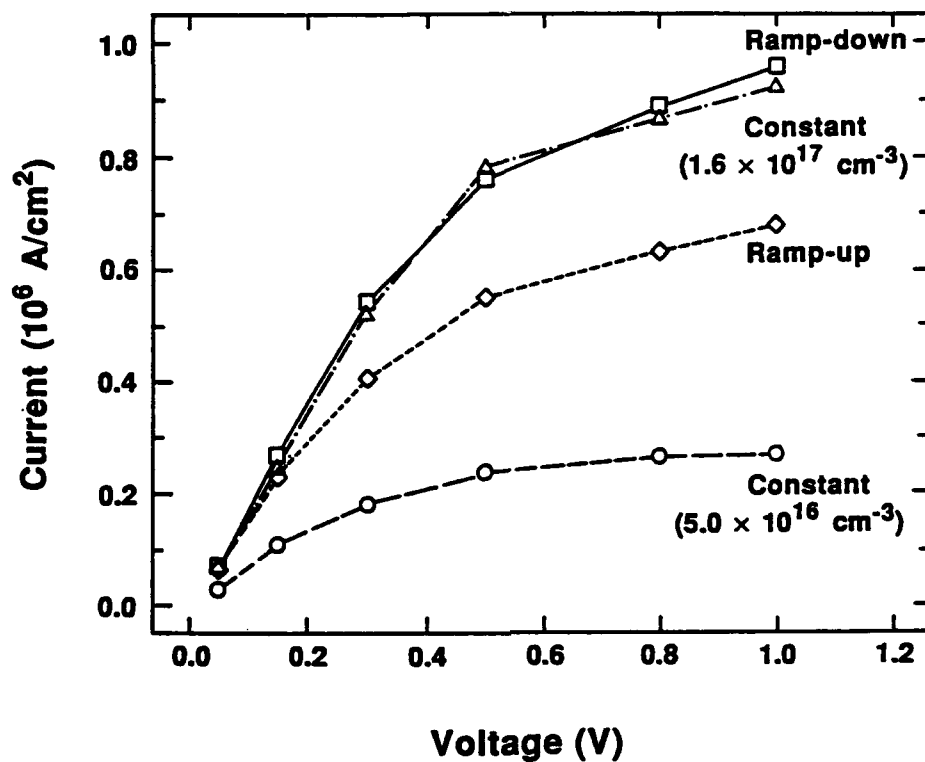
Figure 10: Current-voltage characteristics for ramp-doped n⁺–n–n⁺ structures. The doping density varies linearly between 5×10^{16} cm⁻³ and 5×10^{17} cm⁻³. Simulation results for n⁺–n–n⁺ structures with constant n doping densities of 5×10^{16} cm⁻³ and 1.6×10^{17} cm⁻³ are included for comparison.
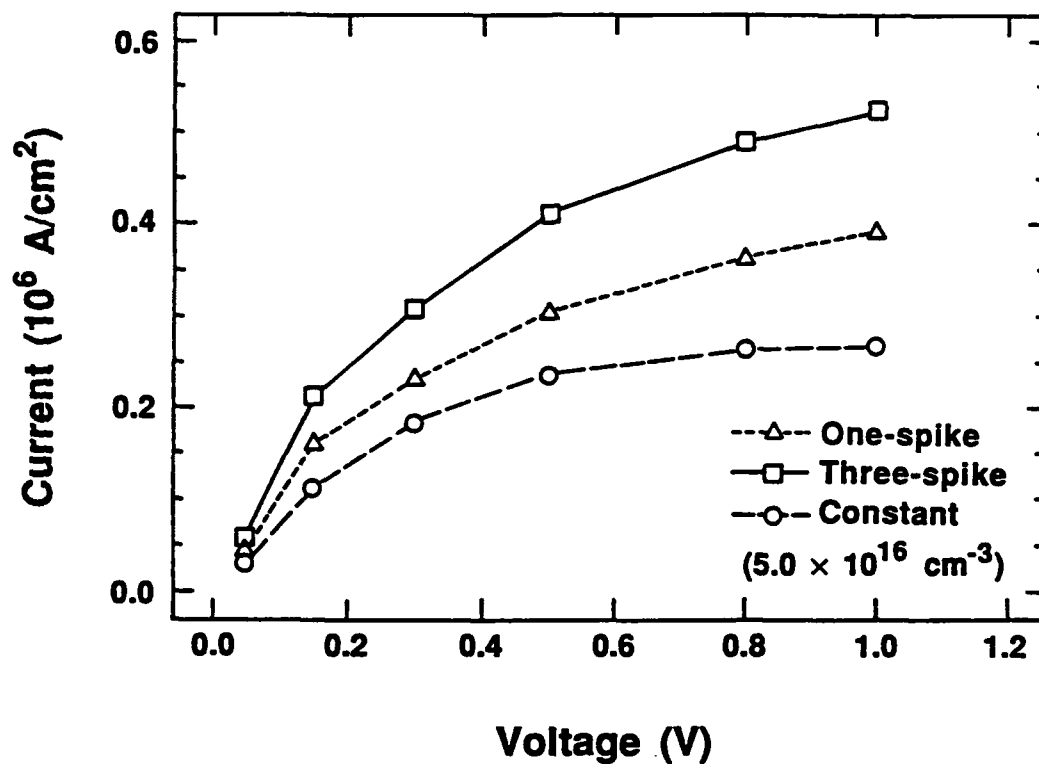
Figure 11: Current-voltage characteristics for one-spike, three-spike, and constant (5×10^{16} cm^{-3}) doped n$^+$–n–n$^+$ structures. The doping densities of the n$^+$ spike(s) and the background are 9.16×10^{17} cm^{-3} and 5×10^{16} cm^{-3}, respectively. The one-spike structure has the n$^+$-spike placed in the center of the n region.

2.2.3 Modeling of hot electrons in silicon devices

For the past fifteen years, the silicon MOSFET industry has been dealing increasingly with problems related to hot electron injection into the oxide with production mode devices. For even longer, laboratories have been measuring and modeling hot electron injection into the oxides with various levels of success [25]. Frequently, the model of choice has been the "lucky electron" model coupled with a drift-diffusion simulator. While the "lucky electron" model has enjoyed a reasonable amount of success, we have recently entered the regime [26] where drift-diffusion simulation is no longer accurate. With this reality, researchers have increasingly been forced to switch to hydrodynamic and Monte Carlo simulators to better predict the behavior of devices. Using these models (especially Monte Carlo), significantly more information about the electron energy distribution is available, giving us the opportunity to improve upon the "lucky electron" model. Full theoretical treatment of the entire hot electron injection condition poses many serious technical difficulties [27] but some first pass efforts [28] indicate we may have a reasonable hope for success. We can then couple these injection characteristics with the oxide trapping characteristics [29,30] to give us a second generation model to supplant the "lucky electron" model.

Within the past year, we have developed a state-of-the-art Monte Carlo simulator of electrons for silicon devices. This simulator uses a realistic band structure (derived from pseudopotential calculations) for the best accuracy in simulating band effects on electron simulation. It also uses an ensemble method of modeling which allows the simulation to account for both spatial and electron-electron intercollisional effects in a self-consistent manner. In addition, our Monte Carlo model includes all of major scattering mechanisms important for silicon simulation. These mechanisms are acoustic phonon, intervalley phonon, impact ionization, ionized impurity and electron-electron scatterings. This rather accurate implementation of physical details results in a reasonable field vs. velocity and scattering rates which compare favorably with the full numerical calculations of Fischetti [31].

In order to accurately model complex device structures, we have also developed a non-uniform mesh Poisson solver which is re-evaluated at frequent time intervals to reflect changes in the potential distribution due to the movement of the electrons in the simulation. This movement is mirrored in the calculation of background hole concentrations. The carrier concentrations remain self-consistent by updating the hole concentrations using the quasi-Fermi level derived from the Poisson solution. At the same time, an efficient method has been implemented which allows to transfer PISCES-modeled and developed structures into one of our Monte Carlo runs. This approach will improve overall computing time and efficiency significantly by providing a smart initial guess and, thus, will permit us to concentrate to the regimes of sensitivity in a greater detail.

Calculations of actual MOSFET structures is now finishing the debugging stage and the preliminary data begin to sh ∴ ⅃ₑ importance and value of our model in the study of hot electron effects and the related aging issues in these devices. Figure 12 demonstrates that electrons experience a significant velocity overshoot region even at reasonably long channels (1 μm) when stressed at high voltages (V_d=6 V, V_g=3 V, V_s=V_b=0 V). The electron energy distribution tail in the drain pinch-off region is also seen to have a significant population beyond the 3.1 eV necessary to inject electrons into the oxide as shown in Fig. 13. Such details are the essential information to understand nonlinear electron transport in submicron devices. We expect to obtain more data in our effort to develop a realistic model for oxide trapping and the generation of interface states at the Si/SiO$_2$ interface within the next few weeks.

2.3 Publications and Presentations

During the last year we have made six oral presentations at national and international conferences. Also, twelve written manuscripts have been published in the refereed literature. In addition, another manuscript has been accepted for publication and six manuscripts have been submitted or are currently in preparation. The following paragraphs summarize the presentations and publications made
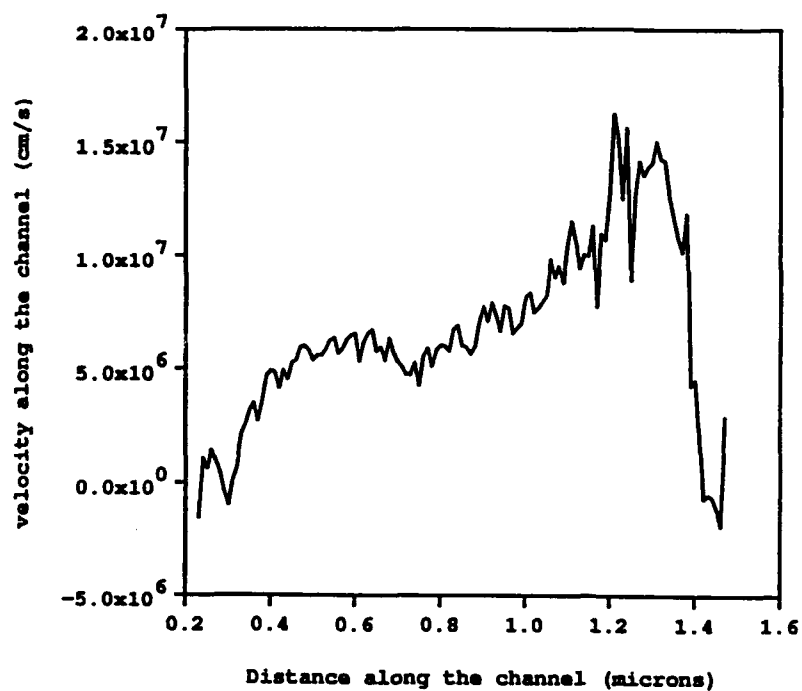
Figure 12: Calculated electron velocity along the channel in a 1-μm gate-length MOSFET at high voltages (V_d=6 V, V_g=3 V, V_s=V_b=0 V).
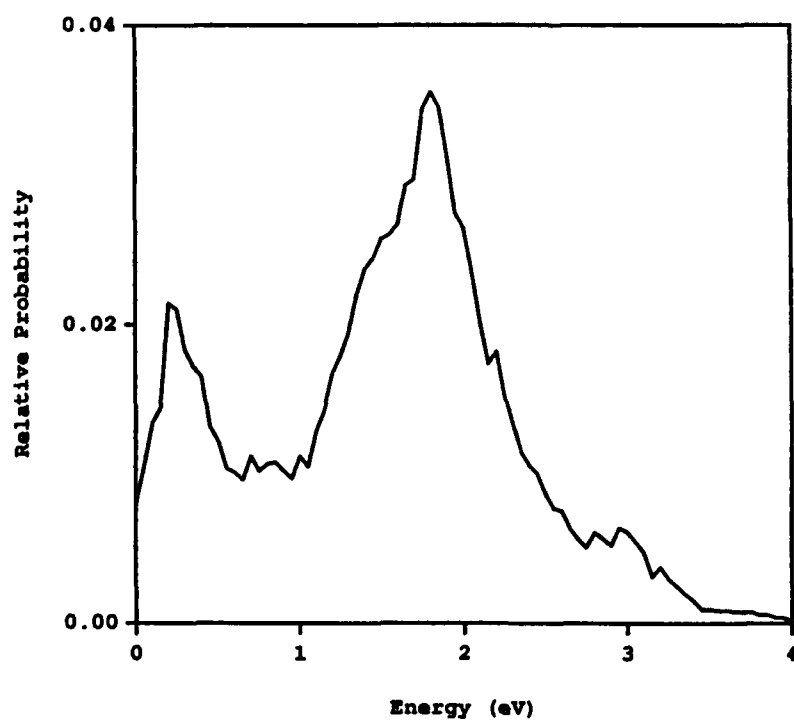

Figure 13: Calculated electron energy distribution along the channel for the same device and bias conditions as in Fig. 12.

under this program during the last year, and include material not previously reported to ONR in the last annual report as well as material which was accepted for publication in 1991 and has since been published in 1992.

A. *Conference Presentations and Seminars*

D. L. Woolard, H. Tian, M. A. Littlejohn, R. J. Trew, and K. W. Kim, "Impact of Electron K-Space Transfer and Band Nonparabolicity on Velocity Overshoot in GaAs Devices," presented at the 7th Intl. Conf. on Hot Carriers in Semiconductors, (July, 1991, Nara, Japan).

D. L. Woolard, R. J. Trew, M. A. Littlejohn, and C. T. Kelly, "A Study of Electron Transit Time in Ballistic Diodes Using a Multi-Valley Hydrodynamic Transport Model," presented at the 13th Biennial IEEE/Cornell University Conf. on Advanced Concepts in High Speed Semiconductor Devices and Circuits (August, 1991, Ithaca, New York).

U. K. Mishra, L. M. Jelloian, M. Lui, M. Thompson, S. E. Rosenbaum, and K. W. Kim, "Effect of n and p Channel Doping on the I-V Characteristics of AlInAs-GaInAs HEMTs," presented at the 18th Intl. Symp. on Gallium Arsenide and Related Compounds (September, 1991, Seattle, Washington).

H. Tian, K. W. Kim, and M. A. Littlejohn, "Ensemble Monte Carlo Study of A Novel Heterojunction Real-Space Transfer Logic Transistor (RSTLT)," presented at the IEEE Intl. Electron Devices Meeting (December, 1991, Washington, DC).

D. L. Woolard, T. A. Winslow, M. A. Littlejohn, and R. J. Trew, "An Extended Scharfetter-Gummel Algorithm Suitable for Solving a Nonparabolic Hydrodynamic Transport Model," presented at the 8th Intl. Conf. on the Numerical Analysis of Semiconductor Devices and Integrated Circuits (NASECODE VIII) (May, 1992, Vienna, Austria).

H. Tian, K. W. Kim, M. A. Littlejohn, U. K. Mishra, and M. Hashemi, "Ensemble Monte Carlo Simulation of Electron Transport in GaAs N^+–N–N^+ Structures with Laterally Varying Doping," presented at the 8th Intl. Conf. on the Numerical Analysis of Semiconductor Devices and Integrated Circuits (NASECODE VIII) (May, 1992, Vienna, Austria).

B. *Refereed Publications, Papers Accepted for Publication, and Papers in Preparation*

H. Tian, K. W. Kim, and M. A. Littlejohn, "An Investigation of Doping Profile Variations on AlGaAs/GaAs High Electron Mobility Transistor Performance," J. Appl. Phys. 70, 4593 (1991).

L. F. Register, M. A. Littlejohn, and M. A. Stroscio, "Path-Integral Monte Carlo Calculation of Free and Confined Carrier Real Self-Energies at Non-Zero Temperatures," Superlatt. Microstruct. 10, 47 (1991).

D. L. Woolard, H. Tian, R. J. Trew, M. A. Littlejohn, and K. W. Kim, "A New Hydrodynamic Electron Transport Model: Nonparabolic Corrections to the Streaming Terms," Phys. Rev. B 44, 11119 (1991).

D. L. Woolard, R. J. Trew, M. A. Littlejohn, and C. T. Kelly, "A Study of Electron Transit Time in Ballistic Diodes Using a Multi-Valley Hydrodynamic Transport Model," Proceedings of the 13th Biennial IEEE/Cornell University Conf. on Advanced Concepts in High Speed Semiconductor Devices and Circuits, pp. 131-140, 1991.

D. L. Woolard, H. Tian, M. A. Littlejohn, R. J. Trew, and K. W. Kim, "Impact of K-Space Transfer and Band Nonparabolicity on Electron Transport in a GaAs Ballistic Diode," Semicond. Sci. Technol. 7, B354 (1992).

H. Tian, K. W. Kim, and M. A. Littlejohn, "Ensemble Monte Carlo Study of A Novel Heterojunction Real-Space Transfer Logic Transistor (RSTLT)," IEDM Tech. Digest, pp. 515-518, 1991.

D. L. Woolard, T. A. Winslow, M. A. Littlejohn, and R. J. Trew, "An Extended Scharfetter-Gummel Algorithm Suitable for Solving a Nonparabolic Hydrodynamic Transport Model," Proceedings of NASECODE VIII, pp. 54-55, 1992.

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H. S. Kim, H. Tian, K. W. Kim, and M. A. Littlejohn, "Electron Velocity-Field Characteristics of $In_{0.52}Al_{0.48}As$," Appl. Phys. Lett. 61, 1202 (1992).

H. Tian, K. W. Kim, M. A. Littlejohn, U. K. Mishra, and M. Hashemi, "Effects of Doping Variations on Electron Transport in GaAs n^+-n-n^+ Structures," accepted for publication in J. Appl. Phys.

T. Kaneto, K. W. Kim, and M. A. Littlejohn, "A Comparison of Minority Electron Transport in $In_{0.53}Ga_{0.47}As$ and GaAs," submitted to Appl. Phys. Lett.

H. Tian, K. W. Kim, and M. A. Littlejohn, "Ensemble Monte Carlo Study of Novel Charge Injection Transistors (CHINTs) with Engineered Heterojunction Source (Launcher) and Drain (Blocker) Configurations," submitted to Appl. Phys. Lett.

J. J. Ellis-Monaghan, K. W. Kim, and M. A. Littlejohn, "Monte Carlo Modeling of Hot Electron Injection into SiO_2 as Correlated to Charge Pumping Measurements," in preparation, to be submitted to IEEE Trans. Electron Devices.

H. Tian, K. W. Kim, M. A. Littlejohn, and U. K. Mishra, "Influence of Channel Doping on 0.25 μm

Channel-Length AlInAs/GaInAs High Electron Mobility Transistor Performance," in preparation, to be submitted to IEEE Electron Device Lett.

D. L. Woolard, T. A. Winslow, M. A. Littlejohn, and R. J. Trew, "Application of an Extended Scharfetter-Gummel Algorithm to Solving a Nonparabolic Hydrodynamic Transport Model," in preparation, to be submitted to IEEE Trans. Electron Devices.

D. L. Woolard, H. Tian, M. A. Littlejohn, and K. W. Kim, "A Monte Carlo Investigation of Electron Distributions and Thermal Energy Flow in GaAs Ballistic Diode Structures," in preparation, to be submitted to J. Appl. Phys.

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Appendix A

LIST OF REFEREED PUBLICATIONS ON THIS PROGRAM SINCE 1975

1. M. A. Littlejohn, J. R. Hauser, and T. H. Glisson, "Monte Carlo Calculation of Transport Properties of GaN," Appl. Phys. Lett. 26, 625 (1975).

2. J. R. Hauser, M. A. Littlejohn, and T. H. Glisson, "Velocity-Field Relationship for InAs-InP Alloys Including the Effects of Alloy Scattering," Appl. Phys. Lett. 28, 458 (1976).

3. J. W. Harrison and J. R. Hauser, "Theoretical Calculations of Electron Mobility in Ternary III-V Compounds," J. Appl. Phys. 47, 292 (1976).

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7. M. A. Littlejohn, J. R. Hauser, T. H. Glisson, and L. A. Arledge, "High Field Transport and MESFET Performance in Ternary and Quaternary III-V Semiconductors," Proceedings Sixth Biennial Cornell Electrical Engineering Conf.: Active Microwave Semiconductor Devices and Circuits, Cornell University, Ithaca, NY, pp. 55-64, August, 1977.

8. T. H. Glisson, J. R. Hauser, M. A. Littlejohn and Williams, "Energy Bandgap and Lattice Constant Contours of III-V Quaternary Alloys," J. Electron. Mater. 7, 1 (1978).

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Appendix B

This appendix contains the title page of each paper published in the refereed literature which were supported on the ONR project during the 1991-1992 contract period. Copies of these papers have been sent to the program manager under separate cover. A list of these papers is included below.

1) H. Tian, K. W. Kim, and M. A. Littlejohn, "An Investigation of Doping Profile Variations on AlGaAs/GaAs High Electron Mobility Transistor Performance," J. Appl. Phys. 70, 4593 (1991).

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An investigation of the effects of doping profile variations on AlGaAs/GaAs high electron mobility transistor performance

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We present results from a theoretical study of the influence of doping profile variations on the performance of delta-doped AlGaAs/GaAs high electron mobility transistors (HEMTs). An ensemble Monte Carlo simulation coupled with a self-consistent solution of the two-dimensional Poisson equation is used to investigate HEMTs which employ both single and double delta-doped profiles with varying doping configurations. The calculated results reveal that single delta-doped HEMTs designed with identical threshold voltages exhibit improved device behavior when thinner delta-doped layers with more heavily doped concentrations are utilized. For double delta-doped HEMTs with an identical total doping in the AlGaAs layer, improved threshold voltage control is obtained as the spacing between two delta-doped layers increases. However, this increase in spacing also causes a degradation in transconductance, cut-off frequency, and switching time. As gate bias increases, the dependence of device performance (or degradation) on the spacing between doping planes becomes less pronounced due to the upward shift in threshold or "onset" of parallel conduction in the AlGaAs layer.

I. INTRODUCTION

The high electron mobility transistor (HEMT) was first developed in 1980[1] and, today, the AlGaAs/GaAs HEMT remains as one of the most important heterojunction structures due to its excellent device performance, the maturity of the materials growth technology, and the excellent lattice match for the AlGaAs/GaAs material system. Further device improvements are needed in order to fully exploit the potential of AlGaAs/GaAs HEMT structures. Unfortunately, improvements in "conventional" uniformly doped HEMTs are limited by the occurrence of persistent photoconductivity,[2] threshold voltage shift,[3] and collapse of current-voltage (*I-V*) characteristics[4] due largely to effects caused by *DX* centers and surface states. The use of low Al mole fraction can reduce these effects; however, this also reduces the conduction-band edge discontinuity, resulting in decreased channel electron density and degraded device performance. This inherent limitation can be circumvented by device structure modifications, such as those employed in delta-doped (also referred to as pulse-doped or planar-doped) AlGaAs/GaAs HEMT structures. Recently, delta-doped HEMTs have attracted much attention. Experiments show that these devices achieve improved threshold control, high channel electron density, reduced trapping effects, and high breakdown characteristics.[5-10]

Detailed investigations of delta-doped HEMTs are necessary to reveal and understand the underlying device physics. While extensive study of conventional uniformly doped HEMTs has been reported,[11-18] the theoretical investigation of delta-doped HEMTs is rare.[8,9,19] The operation of submicron delta-doped HEMTs involves nonstationary electron transport and real-space transfer effects.[17-21] Also, the degeneracy effect, *DX* centers and surface states have significant influence on practical device operation.[19-24] Therefore, the development of more accurate and complete device models must include these effects. Furthermore, it is important to explore new approaches which can lead to improvements in AlGaAs/GaAs HEMTs. Specifically, reducing series resistance and increasing current drive capability of the single delta-doped HEMT structure is of importance for microwave and power applications. As an alternative, a structure with a second delta-doped layer introduced in the AlGaAs layer (i.e., a double delta-doped HEMT) could be used. This structure, while unavailable experimentally, merits study since the introduction of a second delta-doped layer could possibly provide more drive current and reduce source-gate and gate-drain series resistance without reducing the advantages provided by single delta doping. A double delta-doped structure can be realized by molecular-beam epitaxy or metalorganic chemical vapor deposition technologies. However, a theoretical study can provide guidance for the experimentalists to assess the performance of such a device and its dependence on doping parameters and bias conditions.

With these motivations, we employ physical device models to examine the effects of doping profile variations on the performance of two sets of HEMT devices. The first set includes single delta-doped HEMTs with varying doping configurations and constant threshold voltage. Also, for the first time, an attempt is made to analyze the performance of proposed double delta-doped HEMTs. This second set of devices is studied by varying the spacing between two delta-doped layers with identical widths and total doping concentrations. Device performance is examined in terms of threshold voltage control, transconductance, cut-off frequency, and characteristic switching times. [Since the main purpose of this work is to study the

PATH-INTEGRAL MONTE CARLO CALCULATION OF FREE AND CONFINED CARRIER REAL SELF-ENERGIES AT NON-ZERO TEMPERATURES

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A *path-integral Monte Carlo* method for calculation of real self-energies of free and confined carriers at non-zero temperatures is presented. An efficient numerical method for calculating the polar-optical phonon *influence functional* has been developed and incorporated into a previously developed PIMC for calculating equilibrium properties of uncoupled carriers. As illustrative examples, calculations of carrier real self-energies are performed for bulk *GaAs* as a function of temperature, and for *AlGaAs-GaAs*-like square quantum wires at 77K and 300K as a function of wire width. The self-energies obtained here, in part, represent new results for these systems. Where previous results are available, the agreement is good.

1. Introduction

The *Feynman path-integral (FPI)* formulation of quantum mechanics allows formal inclusion of carrier phonon coupling to all orders in the coupling potential [1,2]. For this reason the FPI formalism long has been used to analytically calculate carrier real self-energies and effective masses in bulk semiconductors [3–6]. However, extension of the FPI formalism to analytic study of ultrasmall devices has been hindered by approximations required to model confined geometries [7]. Previously, though improved results were not obtained, it was demonstrated that carrier self-energies in bulk semiconductors at 0K could be calculated using numerical *Path-Integral Monte Carlo (PIMC)* methods as well [8–10]. However, to the best of the authors' knowledge, these calculations were not extended to nonzero temperatures or confined de-

*Current address

vice geometries. Here, a PIMC method for calculating free and confined carrier self-energies at non-zero temperatures is presented.

2. Feynman Path-Integral Formalism

In the FPI formalism, for a coupled carrier-phonon system, the equilibrium density matrix for the carrier averaged over the phonon coordinates and subject to a Maxwell-Boltzmann distribution in energies at temperature T is given by

$$\rho(\vec{r},\vec{r}';T) = \int_{\vec{r}'}^{\vec{r}} \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar/k_B T}\left[\tfrac{1}{2}m^*|\dot{\vec{r}}(t)|^2 + V[\vec{r}(t)]\right]dt\right\}$$
$$\times \mathcal{F}[\vec{r}(t)]\,\mathcal{D}\vec{r}(t).$$

(1)

Here, the "$\int_{\vec{r}'}^{\vec{r}}...\mathcal{D}x(t)$" signifies an integral over all paths from $\vec{r}'$ to $\vec{r}$ that are continuous functions of time, and $\mathcal{F}[\vec{r}(t)]$ is the *influence functional* that accounts for

Hydrodynamic electron-transport model: Nonparabolic corrections to the streaming terms

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This paper presents a hydrodynamic model suitable for studying hot-electron transport in semiconducting materials with nonparabolic conduction bands. The model presented is based upon a unique derivation of the moments of the Boltzmann-transport equation for the streaming (collision-independent) terms. This derivation implements an efficient and compact mathematical formalism appropriate for electrons under the influence of high electric fields and nonstationary conditions. The theoretical investigation also introduces a distributional form with nonparabolic properties to precisely define the resulting nonparabolic *streaming* parameters. The final set of model equations is exhibited in a fashion to clearly show the correction factors to the more familiar hydrodynamic model applicable for the constant-effective-mass case. In general, the hydrodynamic (or conservation) model contains *pure transport* terms that are treated as being independent of the specific dissipation mechanisms and *collision* terms to directly account for the influence of scattering. Since the collision terms are *almost* always treated phenomenologically using a relaxation-time approximation, our formulation of the streaming terms should significantly improve the overall accuracy of the approach. In addition, this paper presents the results of an extensive investigation of the assumed ansatz distribution and resulting nonparabolic-model parameters using an elaborate Monte Carlo model. The Monte Carlo technique was used to generate comparison electron distributions and exact values for the nonparabolic transport parameters for stationary and nonstationary electronic structures. In all cases, excellent agreement was found between the Monte Carlo–calculated parameters and the derived nonparabolic-model terms. The Monte Carlo calculations also revealed that the ansatz distribution used in the derivation represented a significant improvement over the more familar displaced Maxwellian. Therefore, this model should prove very valuable for studying electronic-device structures operating under high-bias conditions.

I. INTRODUCTION

During the past two decades there has been an increased use of hydrodynamic conservation models to investigate nonstationary and nonequilibrium electron dynamics in submicrometer semiconductor devices.[1-14] These models, referred to by some[15,16] as the hydrodynamic equations due to their similarity to the Euler equations of fluid dynamics[17,18] used in classical hydrodynamics studies, are based upon higher moments of the Boltzmann-transport equation (BTE). The popularity of the hydrodynamic electron transport theory is due to the physical and practical attributes of the approach. The hydrodynamic models have the capability to include nonstationary and hot-electron effects[19] and hence are superior to simple drift-diffusion (extreme thermal equilibrium approximation[20] and local-electric-field-dependent case) models. While Monte Carlo methods that solve the full BTE can easily incorporate complicated band structures and detailed scattering rates, hydrodynamic models require much less computation time to generate solutions and possess macroscopic terms which offer important physical insight. Thus the hydrodynamic approach offers much flexibility for future theoretical electron device studies.

Stratton[20] introduced the general conservation or momentum-energy balance approach to investigate hot-electron transport in semiconductors. The analysis performed by Stratton utilized a spherical harmonic expansion with the relaxation-time approximation to define a nonequilibrium distribution which was only slightly anisotropic. This analysis replaced the nonequilibrium distribution by a Maxwellian distribution function in some terms of the BTE. Thus some of the streaming terms in the final transport equations were suppressed. Blotekjaer[21] extended the theory, using a more general analysis which retained all terms of the moment equations, and derived relations applicable to a two-valley semiconductor. These previous investigations were applicable to semiclassical transport and assumed homogeneous materials with parabolic conduction bands.

Since the early work of Stratton and of Blotekjaer, the hydrodynamic approach has been utilized extensively to study various transport phenomena in many different Si,[6,9,22] GaAs,[1,23,24] and heterostructure[11,25,26] electron devices. The particular material, device configuration, and bias conditions under consideration have led to a variety of acceptable simplifications and to a hierarchy of approximate electron-transport models (for example, see Sandborn, Rao, and Blakely[27] and references therein). Also, much effort has been directed toward developing numerical techniques to solve the hydrodynamic transport model self-consistently with Poisson's equation for many semiconductor structures. This has included methods for solving the problem with and without time dependency and in multiple space dimensions[28-30] as well

A Study of Electron Transit-Time in Ballistic Diodes Using a Multi-Valley Hydrodynamic Transport Model

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Abstract

A new multi-valley hydrodynamic transport model has been used to investigate electron transit time through submicron GaAs electron device structures. The study was performed to determine the feasibility of utilizing the velocity overshoot effect in reducing the overall transit time. This new model, which incorporates a separate set of hydrodynamic equations for each conduction band valley (Γ, L and X) and allows for electron exchange through energy dependent relaxation parameters, is applied to a novel structure which reduces upper valley occupancy and enhances device transit time. The results of this study indicate that while velocity speed-up is minimal in the neighborhood of the active (low-doped) region that the velocity overshoot can be extended into the collector region (high-doped) region with significant transit time enhancement.

Introduction

In recent years, a great interest has developed in utilizing velocity overshoot in both GaAs homojunction and heterojunction BJT's to achieve lower electron transit times and hence higher operating frequencies[1, 2, 3]. Investigations of these devices have shown the emitter-collector transit time (τ_{ec}) and the collector transit time (τ_c) to be dominant factors in determining the total transit time[4]. This fact has directed much energy in the simulation and modeling communities toward designing and studying electronic structures which would reduce these figures of merit (τ_{ec} and τ_c). In fact, there have been many theoretical results [5, 6, 7] which indicate that velocity overshoot can be exploited, by select designs and proper biases, to achieve very efficient high frequency devices. However, questions have been raised as to whether conventional device structures can exhibit such enhanced effects. Also, simulation evidence has been reported to indicate that velocity overshoot may be over estimated in such structures[8].

In this paper, a new multi-valley hydrodynamic transport model is used to investigate the feasibility of utilizing the velocity overshoot effect in reducing electron transit time through submicron GaAs electronic device structures. In previous work [9, 10], a novel approach has been presented to incorporate conduction band nonparabolicity into the hydrodynamic model. However, for this initial investigation with the new multi-valley model, which incorporates a separate set of hydrodynamic equations for each conduction band (Γ, L and X) and allows for electron exchange through energy dependent relaxation parameters, the nonparabolic correction terms will be suppressed. This was done to simplify the analysis and to provide a base for future nonparabolic studies. Additional features of the model include self-consistent potentials and realistic boundary conditions.

Impact of *k*-space transfer and band non-parabolicity on electron transport in a GaAs ballistic diode

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Abstract. In this paper, the results of studying a submicron GaAs ballistic diode, using a new multi-valley (Γ, L and X) non-parabolic hydrodynamic transport model, are presented. Numerical simulations indicate that accurately including the effects of non-parabolicity in the streaming terms and *k*-space transfer in the velocity and energy equations is very important in correctly determining the conductance of the device. The existence and amount of negative differential conductance was determined to be strongly influenced by both of these physical factors. Furthermore, the sensitivity of device conductance to changes in the thermal conductivity is diminished significantly when non-parabolicity is accurately incorporated.

1. Introduction

Advanced macroscopic transport models, based upon moments of the Boltzmann transport equation (BTE) as opposed to a full microscopic description (e.g., the Monte Carlo (MC) approach), are valuable tools to *efficiently* investigate electron dynamics in submicron semiconductor structures [1]. However, these models must accurately reflect non-equilibrium and non-stationary electron physics before they can be applied successfully to a wide variety of device operating conditions. Presently, the majority of macroscopic electron device models treat the multi-valley problem indirectly (effective single-electron gas approximation) and ignore the full effects of band non-parabolicity [2]. When more complete macroscopic models are implemented, they sometimes predict questionable results. For example, a two-valley (parabolic) hydrodynamic model has been used to derive negative differential conductance in a GaAs FET while corresponding MC simulations indicate no such effect [3].

In this paper, a new hydrodynamic transport model (HTM) suitable for studying hot electron transport in multiple non-parabolic conduction bands is investigated. The impact of *k*-space (intervalley) transfer and band non-parabolicity is examined by studying variations of this HTM. To determine the influence of these effects individually, these various forms of the model were applied to a submicron GaAs ballistic diode. Numerical simulation results indicate that including the effects of non-parabolicity in the streaming terms and intervalley scattering in the velocity and energy equations strongly influences the characteristics of the device in the non-linear (saturation) region. These results demonstrate that

correctly including non-parabolicity effects in the hydrodynamic model reduces the amount of negative differential resistance (NDR). Also, the amount of NDR was found to be less sensitive to changes in the thermal conductivity when non-parabolicity is accurately incorporated. Therefore, these results verify the importance of both non-parabolicity and intervalley effects in the HTM.

2. The hydrodynamic transport model

For these studies, a submicron GaAs ballistic diode (see inset in figure 1) will be considered with transport in each
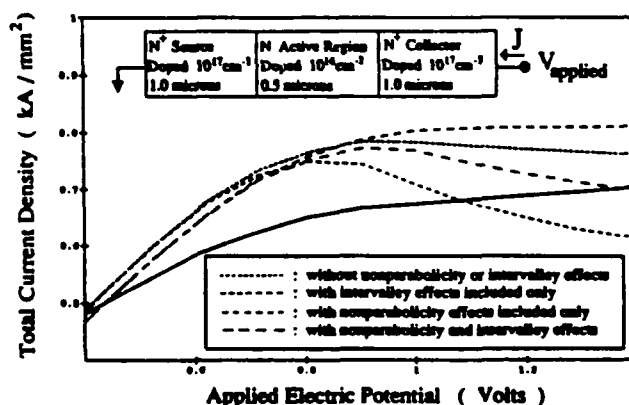

Figure 1. Total electron current density against applied electric potential for a submicron GaAs ballistic diode (see inset). Results are for variations in the HTM (broken curves) and a MC study (full curve). Here $g = 1$ in the HTM.

ENSEMBLE MONTE CARLO STUDY OF A NOVEL HETEROJUNCTION REAL-SPACE TRANSFER LOGIC TRANSISTOR (RSTLT)

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ABSTRACT

A novel real-space transfer logic transistor (RSTLT) is proposed based on the real-space transfer of hot electrons in a four-terminal heterojunction microstructure. Self-consistent steady-state and transient Monte Carlo simulations demonstrate that the RSTLT features both logic flexibility and ultra-fast switching speed. Calculated results show that the proposed RSTLT realizes NOT and EQUIVALENT logic functions in a single heterojunction device and a conservative estimate of the characteristic switching time is ~ 3 psec.

INTRODUCTION

Real-space transfer (RST) [1] is the thermionic emission of hot electrons (from one semiconductor layer) over heterointerface barriers to different semiconductor layers. Successful implementations of the RST concept have been demonstrated by experimental realizations of the negative resistance field-effect transistor (NERFET) [2], charge injection transistor (CHINT) [3] in both AlGaAs/GaAs and InGaAs/InAlAs material systems, and real-space transfer transistor (RSTT) [4] using strained InGaAs/AlGaAs/GaAs layers. Promising performances have been achieved in these devices, with reported values of transconductance exceeding 2300 mS/mm [3] and unity-current gain frequency of 60 GHz [4] at room temperature. Also, a NORAND functional element based on a multi-terminal CHINT structure has been proposed recently [5], demonstrating the potential logic applications of real-space transfer devices. In this work, we propose a novel logic circuit element - the real-space transfer logic transistor (RSTLT). The operation of this proposed microstructure is based on the concept of hot electron real-space transfer and the fact that the spatial location of electron RST is determined by applied bias and heterointerface energy barrier height. Self-consistent ensemble Monte Carlo simulations are used to theoretically 'build' a RSTLT with flexible logic functions and ultra-fast speed.

RSTLT STRUCTURE AND SIMULATION METHOD

Figure 1 shows the proposed RSTLT structure. The device has two separate collectors (C1 and C2) as output terminals which are connected through load elements (R) to the positive power supply (V_C), a drain (D) input terminal and a common source (S) terminal which is at ground potential. When D is biased at logic low (positive logic), channel electrons confined in the potential well between the channel-barrier heterointerfaces will not have enough energy to overcome the energy barrier until reaching C2 where they are collected. In this case C1 is logic high and C2 is logic low (terminal voltages of C1 and C2 are high and low, respectively). On the other hand, if D is high, most electrons gain sufficient energy to overcome the barrier while passing under C1. Therefore, C1 becomes low and C2 high. Thus, the RSTLT realizes the logic NOT (C1) and EQUIVALENT (C2) functions of the input control signal (D), i.e., C1 = $\overline{D}$, C2 = D, as shown in the inset of Fig. 1. In order to ensure
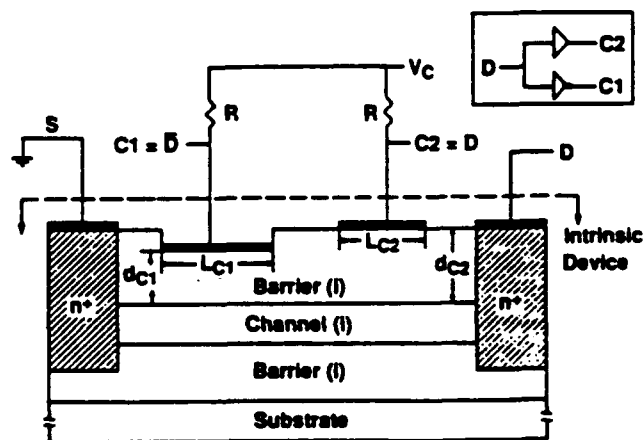

Figure 1. Proposed RSTLT structure. The inset on the top right shows the logic symbol of the structure.

18.6.1

AN EXTENDED SCHARFETTER-GUMMEL ALGORITHM SUITABLE FOR SOLVING A NONPARABOLIC HYDRODYNAMIC TRANSPORT MODEL

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Abstract - This paper presents an *extended* Scharfetter-Gummel current-density discretization formula sufficient for solving an advanced hydrodynamic electron transport model. This improved discretization expression is specifically developed for a new hydrodynamic transport model suitable for studying hot-electron transport in semiconducting materials with nonparabolic conduction bands. While this *extended* formulation properly incorporates many advanced effects associated with hot-electron transport, its *primary feature is the accurate treatment of the convection term* (or displacement energy term) which is present in both conventional (i.e. drifted Maxwellian model) and the advanced nonparabolic model discussed in this paper. Our derivation overcomes nonlinear problems introduced by this convection term and results in an improved expression to approximate current density.

I. INTRODUCTION

At present, Monte Carlo (MC) methods and hydrodynamic transport models (HTM's) are the two most popular approaches utilized to investigate hot-electron phenomenon in submicron structures. While MC methods[1], which solve the full Boltzmann transport equation (BTE), can easily incorporate detailed transport physics, this approach can become impractical in some instances due to the extensive computational requirements. HTM's, which are based upon macroscopic conservation equations derived from moments of the BTE, include nonstationary and hot-electron effects[2] while requiring much less computation time to generate solutions. The physical and practical attributes of HTM's have lead to their extensive application. In turn, advanced HTM's have been developed which are accurate for various device structures and operating conditions[3]. While HTM's represent a considerable reduction in complexity (as compared to solving the full BTE), their solution for arbitrary device structures is still a very formidable mathematics problem. When HTM's are applied self-consistently with Poisson's equation, one must solve a set of nonlinear coupled partial differential equations. This task requires the application of accurate and stable numerical techniques. Since the success of any numerical simulation is critically dependent on convergence rate and numerical stability, the choice of an efficient discretization scheme is very important[4].

It is well known that a central difference approach is not adequate for discretizing the current continuity equation due to the development of oscillations or "*wiggles*" in the solution[5]. To insure numerical stability, Scharfetter and Gummel[5] introduced a physics-based current density formulation for the drift-diffusion (DD) model (i.e. they assumed current density varies weakly with position). The success the Scharfetter-Gummel (SG) scheme, in DD model simulations, has motivated various generalizations of this discretization technique for the hydrodynamic equations[7]. However, most extensions of the SG formula for HTM's either ignore convention terms[4] or else assume a priori that they are defined in a previous step of an iteration procedure[7]. In this paper, an analytical method is presented to develop an extended SG current density formula which directly includes the effects of the nonlinear convention term. This SG algorithm is specifically developed for use in solving a new nonparabolic HTM. Also, the extended formula is compared to one which ignores energy displacement to illustrate the influence of this nonlinear effect on the predicted current density.

II. THE NONPARABOLIC MODEL

Previously, a hydrodynamic model suitable for studying hot-electron transport in semiconducting materials with nonparabolic conduction bands was presented[3]. This new model contains advanced nonparabolic streaming (collision independent) terms which were derived by applying a unique set of moment operators (i.e. orders of nonlinear k-space velocity as opposed to momentum) to the collisionless Boltzmann transport equation. The resulting system of moment (balance) equations were closed (terminated) by introducing an empirical distribution function which accurately approximates the properties of electrons drifting in nonparabolic conduction bands. To treat intervally transfer effects that are present in multi-valley systems (e.g. GaAs), a three-valley (Γ, L and X) ensemble relaxation time model has been developed and implemented[8]. The full multi-valley nonparabolic HTM, with a phenomenological heat flow vector term, consists of the transport equations

$$\frac{\partial n_i}{\partial t} = -\nabla_r(n_i v_i) + \left(\frac{\partial n_i}{\partial t}\right)_{coll.},\tag{1}$$

$$\frac{\partial v_i}{\partial t} = -v_i \cdot \nabla_r v_i + \frac{F}{\hat{m}_i^*} - \frac{1}{n_i m_i^*}\nabla_r \cdot [P_{v_i}], + \left(\frac{\partial v_i}{\partial t}\right)_{coll.},\tag{2}$$

$$\frac{\partial w_i}{\partial t} = -v_i \cdot \nabla_r w_i + F \cdot v_i - \frac{1}{n_i}\nabla_r \cdot (v_i \cdot [P_{w_i}] + q_i + q_i^p) + \left(\frac{\partial w_i}{\partial t}\right)_{coll.}\tag{3}$$

and

$$q_i^p = -Q\frac{4}{9}\frac{\mu_i}{q}n_i w_i \nabla_r w_i\tag{4}$$

for each conduction band valley ($i = \Gamma$, L and X). In the previous model equations, n_i is the electron concentration, v_i is the average electron velocity, w_i is the average electron energy and $F = q\nabla_r \psi$ is the force on the electron. In this HTM, the resulting constitutive relations are: an average effective mass $\hat{m}_i^*(v_i, T_{wi}) = m_i^*(1 + 3\alpha_i k_B T_{wi} + 7.5(\alpha_i k_B T_{wi})^2 + \alpha_i m_i^*|v_i|^2)$, an effective velocity pressure $[P_{v_i}] = (m_i^*/\hat{m}_i^*)n_i k_B T_{wi}[I]$, an effective energy pressure $[P_{w_i}] = n_i k_B T_{wi}(1 + 2\alpha_i k_B T_{wi} + \alpha_i m_i^*|v_i|^2)[I]$, a nonparabolic heat flow vector $q_i = 5\alpha_i(m_i^*/\hat{m}^*)^2(k_B T_{wi})^2(1 + 21\alpha_i(m_i^*/\hat{m}^*)k_B T_{wi})n_i v_i$, and the nonparabolic energy partition relation $w_i = (3/2)k_B T_{eff}(v_i, T_{wi}) + (\hat{m}_i^*(v_i, T_{wi})/2)|v_i|^2$ with an effective temperature of $T_{eff}(v_i, T_{wi}) = T_{wi}(1 + 2\alpha_i k_B T_{wi} + \alpha_i m_i^*|v_i|^2)$. These previous relations, which express the corrected streaming terms as functions of v, w and nonparabolic conduction-band factor α were verified for both stationary and nonstationary transport in GaAs by two independent Monte Carlo simulation studies[3]. Features of this model which differ from the conventional HTM include: (1) a nonconstant average effective mass $\hat{m}_i^*(v_i, T_{wi})$, (2) a distinctly different velocity and energy pressure (i.e. $[P_{v_i}] \neq [P_{w_i}]$), and (3) a first-principles nonzero heat flow vector q_i. In this model, q_i represents the heat flow resulting from the *symmetric component* of the velocity-space electron distribution in nonparabolic bands. Therefore, the Wiedemann-Franz phenomenological heat flow term, q_i^p in Eq. (4), is introduced to account for possible asymmetry of the electron distribution. In this heat flow term, μ_i is the near equilibrium mobility and Q is a multiplicative constant associated with the particular material under consideration. Dissipation and intervalley transfer effects (i.e. last terms in Eqs. (1) - (3)) are included using an ensemble relaxation time model identical in form to the one proposed by Blotekjaer[9]. To complete the model, the various energy-dependent relaxation times for a multi-valley system (GaAs) have been obtained from stationary MC calculations[3].

ENSEMBLE MONTE CARLO SIMULATION OF ELECTRON TRANSPORT IN GaAs $N^+ - N - N^+$ STRUCTURES WITH LATERALLY VARYING DOPING

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Abstract - The effects of laterally varying doping profile on device electron transport properties are studied using self-consistent ensemble Monte Carlo simulations. Significant performance improvement is observed for $N^+ - N - N^+$ structures with ramp-down doping and multi-spike doping profiles in the active N region. The prospects for application of laterally varying doping schemes in field-effect transistor structures are discussed.

The utilization of 'bandgap engineering' has led to a variety of novel improved device structures in the past decade. Successful integration of 'bandgap engineering' with 'doping engineering' provides additional flexibility and new methods for the future development of advanced semiconductor devices. Currently, most semiconductor devices employ techniques that control doping profiles in the vertical dimension (perpendicular to the direction of carrier transport using e.g., uniform doping, modulation doping, and delta-doping). The rapid development of new technologies such as focused ion beams (FIB) makes possible mask-less direct 'writing' of controlled dopants into semiconductors [1]. Thus, the doping distribution can be tailored in the lateral dimension (parallel to the direction of carrier transport). This added degree of freedom for 'doping engineering' can possibly result in novel device structures with improved performance. The purpose of this paper is to present results of a theoretical study of the effects of laterally varying doping profiles on device electron transport properties, which supports this proposition.

In this work, self-consistent ensemble Monte Carlo simulations are performed to investigate the effects of laterally varying doping on electron transport. The Monte Carlo model employs a three-valley (Γ-L-X), nonparabolic band structure coupled with a solver for Poisson's equation. Trajectories of a large number of sample electrons are traced in real space and in momentum space. Relevant scattering mechanisms (polar optical, equivalent and nonequivalent intervalley, ionized impurity, and electron-electron) are included. In addition, the effect of degeneracy for Γ-valley electrons is taken into account by employing an approximate Fermi-Dirac distribution with calculated local quasi-Fermi level and electron temperature [2]. Charge neutrality in a portion adjacent to the electrodes is maintained throughout the simulation, which serves as the criterion for electron injection. Material and energy band parameters for GaAs are the same as those in Ref. [3]. Lattice temperature is assumed to be 300 K. More detailed model description can be found elsewhere [4]. This transport study assesses advantages, differences, and potential applications of different laterally varying doping profiles on device performance. The test device is a GaAs $N^+(0.5\mu m) - N(0.5\mu m) - N^+(0.5\mu m)$ structure with varied doping profile along the direction of electron transport in the N region. In particular, two groups of laterally

varying doping schemes are studied. They are: 1) ramp-doping [i.e., linearly increasing (ramp-up) or decreasing (ramp-down) doping density within the N region], and 2) spike-doping (i.e., introducing one or more N^+ spikes in the N region). In order to have meaningful comparisons among structures which employ different doping profiles, we apply conditions of identical minimum doping density and total integrated dopant in the N region.

Any successful implementation of a lateral doping scheme should result in improved current drive capability. Among all the devices studied, our simulation results reveal that the most significant improvement can be achieved by employing a structure with a ramp-down doping scheme. For the same applied bias, the ramp-down doped structure exhibits more than 50 % overall improvement in current drive capability compared to that for the structure with the ramp-up doping scheme. This is shown in Fig. 1, where current-voltage characteristics of the structures with ramp-up, ramp-down, and constant minimum N doping profiles are given. The conduction band profile (increasing exponentially along the direction of electron transport) generated by the ramp-down doping scheme and the resultant accelerating electric field profile provide favorable electron transport conditions in which electrons accelerate more efficiently. High average electron velocity, low average electron energy, and high Γ-valley electron occupancy are obtained for the ramp-down doped structure. These results indicate that, on average, more electrons in the ramp-down doped structure accelerate while they stay in the Γ valley. Results from spike-doped structures show that introducing an N^+ spike in the active electron transport (N) region brings improved device
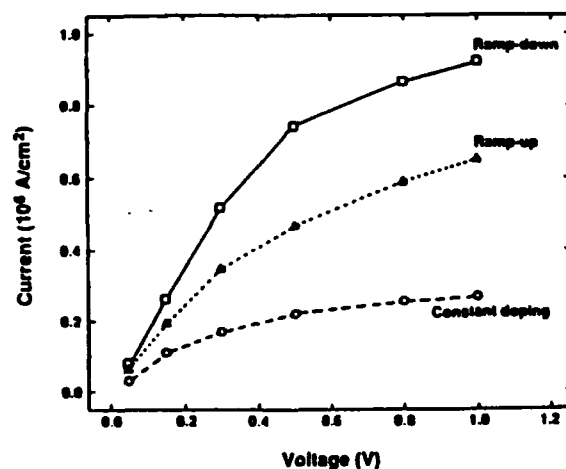

Figure 1. Current-voltage characteristics for the ramp-doped $N^+ - N - N^+$ structures. Doping density varies linearly between $5 \times 10^{16} cm^{-3}$ and $5 \times 10^{17} cm^{-3}$. Result for $N^+ - N - N^+$ structure with constant (minimum) N doping density of $5 \times 10^{16} cm^{-3}$ is included for comparison.

Effect of n and p channel doping on the $I-V$ characteristics of AlInAs–GaInAs HEMTs

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1. Introduction:

Enhancement in the high frequency performance of transistors is dependent
both on improved materials properties and smaller transit distances. This has
resulted in improved performance as devices have progressed from MESFETs
(Wang etal) to GaAs based pseudomorphic HEMTs(Tan etal) to InP based
lattice-matched(Mishra etal, Chao etal) and pseudomorphic(Thompson etal)
HEMTs. The GaInAs based devices have demonstrated the highest speeds
because of a combination of high electron mobility, peak velocity and sheet
charge density in the GaInAs channel of an AlInAs-GaInAs HEMT. The
reduction in gate length to 50 nm has increased the extrinsic f_T of the HEMT
to 292 GHz at room temperature(Thompson etal) but the f_{max} of the HEMT
has been restricted by the rapid increase in the output conductance at the
small gate length. The output conductance is caused by a combination of
substrate injection and channel length modulation. Attempts to reduce the
substrate injection by using a combination of p-doped and wide band gap
buffer layers have had limited success. In this study, we investigate the effects
of doping the channel of an AlInAs-GaInAs modulation doped transistor n
and p type and evaluate the effect on the DC and RF characteristics of devices
with 0.25 μm gate length. Devices with 1 μm gate length were also studied to
determine the gate length dependence. The motivation is to evaluate the
effect of the two doping types on the distribution of electric field in the
channel and study its effect on output conductance and electron transport.
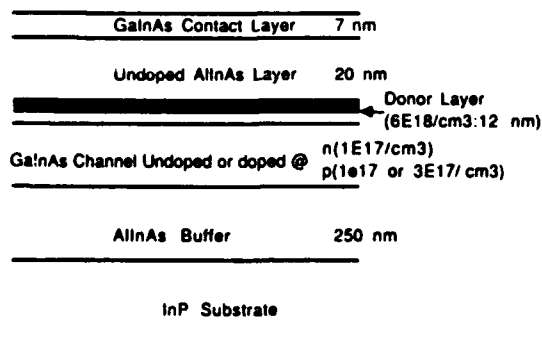

Figure 1: Schematic of the Layer Structures Used in the Study.

Two-Dimensional Analysis of Short-Channel Delta-Doped GaAs MESFET's

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Abstract—Key design parameters for delta-doped GaAs MESFET's, such as delta-doping profile, top layer background doping density, and scaling of lateral feature size, are investigated using a two-dimensional numerical simulation. A three-region (delta-doped conducting channel, top layer, and substrate) velocity–field relation is implemented in the model as appropriate for the particular device structure which is simulated. Simulation results show excellent agreement with our fabricated 0.5-μm gate-length delta-doped GaAs MESFET's based on atomic layer epitaxy material. An extrinsic transconductance of 370 mS/mm and a drain–source current of 270 mA/mm are obtained for typical devices, and the maximum transconductance is as high as 400 mS/mm, which are the best dc results yet reported for 0.5-μm gate-length delta-doped GaAs MESFET's. Considerations of design and optimization are discussed in terms of threshold voltage sensitivity, transconductance, current drive capability, and cutoff frequency, based on both simulation and experimental results.

I. INTRODUCTION

THE DRIVE to achieve high-speed and high-frequency electronic systems has led to continued efforts to develop new device structures. One very promising structure is a field-effect transistor (FET) which incorporates the delta-doping technique. Advanced delta-doped FET structures such as GaAs MESFET's [1]–[4], HEMT's on GaAs [5]–[7] and InP substrates [8], as well as pseudomorphic HEMT's [9] have been demonstrated. The advantages of delta doping in these device structures include high current drive capability, high transconductance, improved threshold voltage control, and improved breakdown characteristics.

Delta-doped GaAs MESFET's based on materials grown by MBE and MOCVD materials have been investigated experimentally by several research groups [1]–[4]. While the results are promising, they also show a wide diversity and fall short of theoretical predictions [1]. The reported maximum transconductance of 0.5-μm gate-length delta-doped MESFET's, for example, ranges from 75 mS/mm [1] to 140 mS/mm [2], to the 400 mS/mm transconductance reported in this paper. Schubert *et al.* [1] studied properties of delta doping in GaAs and predicted that the maximum intrinsic transconductance of a delta-doped MESFET could be higher than that of a comparable AlGaAs/GaAs HEMT in the gate length range of 0.1 to 2.0 μm. Differences between experimental results and theoretical predictions may stem from unknown material properties and differences or uncertainty in processing conditions. On the other hand, design and optimization of such devices play an important role in guiding the improvement of device performance. It is of practical importance to identify the key parameters and the tradeoffs needed for optimized device performance in specific applications.

The intent of this paper is to present a generalized analysis of delta-doped submicrometer MESFET's. We use a two-dimensional drift-diffusion model to simulate the influence of key design parameters on delta-doped MESFET performance. Experimental 0.5-μm gate-length delta-doped MESFET's grown by atomic layer epitaxy (ALE) have also been fabricated. Excellent agreement between simulation and experimental measurement has been obtained. An extrinsic transconductance of 370 mS/mm and a drain–source current of 270 mA/mm are measured for typical devices, while the maximum transconductance is as high as 400 mS/mm. These are the best experimental results yet reported for 0.5-μm gate-length delta-doped GaAs MESFET's. Based on the agreement between simulation results and experimental results for 0.5-μm devices, we then analyze performance dependence on key device parameters and outline some design considerations and tradeoffs for achieving improved delta-doped MESFET operation.

II. DEVICE FABRICATION

A schematic illustration of a delta-doped GaAs MESFET is shown in Fig. 1(a). A very narrow doping profile (Fig. 1(b)) is sandwiched between two undoped (or relatively low-doped) layers. The device structure and the doping profile in the figures are representative of those employed in the experimental device, although the actual device fabricated for measurement in this paper contains a recessed gate. The doping profile used in the simulation

Novel Heterojunction Real-Space Transfer Logic Transistor Structures: A Model-Based Investigation

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Abstract—Ensemble Monte Carlo simulations are employed in order to explore the feasibility of a novel real-space transfer logic transistor (RSTLT) structure. The operational principles of the proposed RSTLT are based on the concept of hot electron real-space transfer (RST), including the fact that the spatial location of electron RST is determined by applied bias and heterointerface energy barrier height in a multiterminal heterojunction microstructure. The results of two-dimensional, self-consistent steady-state and transient simulations demonstrate that the proposed RSTLT features ultrafast current switching which can be used to realize *NOT/EQUIVALENT* logic functions in a single heterojunction device. The logic operation is easily extended to *NOR/AND* functions. A conservative estimate of the characteristic delay time for current switching is ~3 ps in the proposed RSTLT structure.

I. INTRODUCTION

THERMIONIC emission of hot electrons (from one semiconductor layer) over heterointerface barrier(s) to different semiconductor layers in the presence of high electric fields is termed real-space transfer (RST) [1]. Successful implementations of the RST concept have been demonstrated by experimental realizations of the negative resistance field-effect transistor (NERFET) [2]–[4], the charge injection transistor (CHINT) in both AlGaAs/GaAs [5], [6] and InGaAs/InAlAs [7], [8] material systems, and the real-space transfer transistor (RSTT) using strained InGaAs/AlGaAs/GaAs [9] heterostructures. Promising performances in both dc and microwave applications have been achieved in these devices, with reported transconductance values exceeding 2300 mS/mm [6] and unity–current gain frequency of 60 GHz [9] at room temperature. Recently, a CHINT logic element to realize NOR/AND functions [10] has been proposed, demonstrating the potential logic applications of real-space transfer devices. Theoretical investigations of electron transport properties and related device physics in real-space transfer structures have also been performed [11]–

[18]. These studies provide a foundation for device structures with novel operating principles.

It is worth noting that in a real-space transfer device (such as the CHINT), hot electron RST is a *localized* process in which the spatial occurrence of RST is determined by factors such as the device configuration, heterojunction material parameters, and operating bias conditions. This phenomenon has been discussed by interpreting experimental *I–V* characteristics of CHINT structures using positive feedback initiated by a local 'hot spot' in the device channel [8]. Also, Monte Carlo analysis of three-terminal RST devices has indicated the localized nature of electron RST [13]. Recently, we have proposed a novel real-space transfer logic transistor (RSTLT) [19] based on ensemble Monte Carlo studies of hot electron transport in a four-terminal heterojunction microstructure. The operation of the proposed RSTLT is based on the fact that the spatial location of electron RST is determined primarily by applied bias and heterointerface energy barrier height. The dc and transient current switching characteristics of the proposed RSTLT have been discussed briefly [19] (here we define *current switching* as the current exchange among device terminals while transient switching times for the intrinsic device are denoted as *characteristic delay times*). We have demonstrated the the potential logic applications based on multiple terminal current switching characteristics of the RSTLT.

In this work, detailed theoretical investigations using self-consistent, two-dimensional ensemble Monte Carlo simulations are presented which focus on exploring the feasibility of the RSTLT structure in digital applications. The proposed structure differs from the CHINT logic element [10], i.e., the RSTLT employs a different device configuration and terminal arrangement to achieve shorter transient delay time while maintaining logic flexibility. This provides another attractive approach to realize ultrafast multilogic functions in a single heterojunction device. This computer experimental study is used to theoretically "build" a device which allows the logic flexibility and fast speed of available real-space transfer devices to be explored. Electrical characteristics and related device physics of the proposed RSTLT structures are examined in terms of material parameters, device feature size, and bias conditions. In the next section, we de-

Electron velocity-field characteristics of $In_{0.52}Al_{0.48}As$

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Theoretical results of electron transport in n-type $In_{0.52}Al_{0.48}As$ are presented. The transport properties of this important semiconductor were obtained using the Monte Carlo method. In particular, velocity-electric field characteristics for different temperatures and doping concentrations in bulk $In_{0.52}Al_{0.48}As$ are calculated for the first time. Physical parameters for $In_{0.52}Al_{0.48}As$ (which is lattice-matched to InP and $In_{0.53}Ga_{0.47}As$) were obtained based on interpolation of available experimental and theoretical results for InAs, AlAs, and $In_{0.75}Al_{0.25}As$. Our study suggests that $In_{0.52}Al_{0.48}As$ has electron transport properties which are comparable to and complimentary with those of other materials lattice-matched to InP.

Heterojunction devices based on the lattice-matched $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As/InP$ material system have been the focus of extensive experimental studies due to their promising potential for digital, microwave, and optical applications. Impressive device performance has been achieved for the high electron mobility transistor (HEMT),[1] charge injection transistor (CHINT),[2] and semiconductor laser[3] fabricated from this material system. However, certain material-related issues remain which merit careful study if potential applications of these devices are to be fully exploited. As an example, high output conductance has been repeatedly observed in deep-submicron ($\lesssim 0.3$ μm) channel-length HEMTs using the $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As/InP$ material system.[1,4,5] This performance degradation has been suggested to be the result of: (1) electron conduction in the $In_{0.52}Al_{0.48}As$ buffer layer; (2) deep level traps in the top $In_{0.52}Al_{0.48}As$ donor supply layer; and (3) weak impact ionization in the $In_{0.53}Ga_{0.47}As$ channel layer. Studies on the CHINT have also shown that electron transit time in the $In_{0.52}Al_{0.48}As$ collector barrier is the main factor that determines the total device intrinsic delay time.[2] These observations indicate the importance of achieving a better understanding of electron transport in $In_{0.52}Al_{0.48}As$. Unfortunately, there is very little available information on material parameters or electron transport properties for $In_{0.52}Al_{0.48}As$. This is a noticeable void since there have been extensive experimental and theoretical studies of InP and $In_{0.53}Ga_{0.47}As$, and data on $In_{0.52}Al_{0.48}As$ are required in order to perform thorough and more rigorous device simulations in the $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As/InP$ material system.

In this letter, we employ a Monte Carlo model to study electron velocity-electric field characteristics in n-type $In_{0.52}Al_{0.48}As$ for different temperatures and doping concentrations. The set of physical parameters for $In_{0.52}Al_{0.48}As$ required for this study has been obtained based on linear interpolation of available data for the InAs and AlAs binary components, while using the few available (theoretical) material properties of $In_{0.75}Al_{0.25}As$ as a guide. The material parameters which we provide for $In_{0.52}Al_{0.48}As$ and the results of the fundamental electron transport study will serve to promote further experimentation and characterization of $In_{0.52}Al_{0.48}As$-related devices.

The Monte Carlo method used in this work comprises a model for the motion of sample electrons in a three valley (Γ-L-X) semiconductor with nonparabolic analytical band structure under the influence of a uniform applied electric field.[6,7] Relevant scattering mechanisms are polar optical phonon scattering, equivalent and nonequivalent intervalley scattering, ionized impurity scattering, alloy scattering, and impact ionization. In the present work, a single longitudinal-optical (LO) phonon mode is used. There is a possibility that two LO phonon modes due to the InAs-like and AlAs-like vibrations could be active in $In_{0.52}Al_{0.48}As$, since it is known that this condition does exist in some ternary materials. However, this is a subtle point, and detailed properties of the phonon spectra in this material are not sufficiently known at present to justify the use of two LO phonons in the model. The use of a single LO phonon with an energy of 39.5 meV, which was interpolated from local mode energies of 29.6 meV for InAs and 50.1 meV for AlAs, should not detract from the main conclusions of this work.

The ionized impurity scattering rate used in our simulations is based on Ridley's statistical scattering model.[8] In this model, the scattering rate in terms of electron wave vector **k** is given as

$$\frac{1}{\tau_{imp}(\mathbf{k})} = \frac{v_g(\mathbf{k})}{d}\left[1 - \exp\left(-\frac{d}{v_g(\mathbf{k})\tau_{BH}(\mathbf{k})}\right)\right], \quad (1)$$

where $v_g(\mathbf{k})$ is the electron group velocity and $d[=(2\pi N_{dop})^{-1/3}]$ is the average distance between impurities. The electron density is assumed to be equal to the doping concentration (N_{dop}). The scattering rate $1/\tau_{BH}$, which is derived from the Brooks–Herring model,[9] was calculated by following Ruch and Fawcett.[10]

The alloy scattering rate is obtained using[6]

$$\frac{1}{\tau_{alloy}} = \frac{3\pi(m^*)^{3/2}}{8\sqrt{2}\hbar^4}[x(1-x)]\gamma(\epsilon)^{1/2}\frac{d\gamma(\epsilon)}{d\epsilon}\Omega|\Delta U|^2 S(\alpha),$$

$$(2)$$

where ΔU is the alloy scattering potential, x is the alloy composition, Ω is the primitive cell volume, and $\gamma(\epsilon) = \epsilon(1 + \alpha\epsilon)$ for the nonparabolic conduction band. We use the electron affinities of AlAs and InAs to predict a value for ΔU.[6] Here, $S(\alpha)$ is an energy-dependent parameter

Appendix C

The following pages contain brief biographical sketches for Dr. M. A. Littlejohn and Dr. K. W. Kim.

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Education

North Carolina State University	1962	BS	Electrical Engineering
North Carolina State University	1964	MS	Electrical Engineering
North Carolina State University	1967	PhD	Electrical Engineering

Industrial and Academic Experience

1992-present	Director, Southeastern University and College Coalition for Engineering Education (SUCCEED)
1967-present	Assistant Professor/Associate Professor/Professor, Department of Electrical and Computer Engineering, North Carolina State University, Raleigh, North Carolina.
1977-1981 & 1985-1992	Technical Staff Member, U.S. Army Research Office, Research Triangle Park, North Carolina.
1981-1983	Director, Microelectronics Programs, School of Engineering, North Carolina State University, Raleigh, North Carolina.
1984-1985	Associate Dean of Engineering for Research Programs, North Carolina State University, Raleigh, North Carolina.
1988-1989	Associate Director, NSF Engineering Research Center On Advanced Electronic Materials Processing.

Professional Activities

Member of the Advisory Board, IEEE Awards Program For Innovative Educators, 1992- present.

Member at Large, Executive Committee of the Electronics Division of the Electrochemical Society, 1983-1988.

Member, National Academy of Sciences National Research Council Committee on Recommendations for U.S. Army Basic Scientific Research, 1985-1986.

Member, Technical Advisory Board, IEEE Engineering Research and Development Committee, 1986-1989.

Associate Editor, Electronics Division, Journal of the Electrochemical Society, 1987-1990.

Member, NSF Committee on Research Trends and Opportunities for the Metallurgy, Polymers, and Ceramics Section, Division of Materials Research, 1983-1985.

Organizer and Program Chairman, NSF Workshop on The Future of Microstructure Technology, 1985.

Society Memberships and Honors

Institute of Electrical and Electronics Engineers
American Society for Engineering Education
American Physical Society
Electrochemical Society
Certification of Achievement For Patriotic Civilian Service, U.S. Army, 1989
R.J. Reynolds Industries, Inc., Award for Excellence in Teaching and Research, 1983-1987
Alcoa Foundation Distinguished Research Award, 1983

N.C. State University Alumni Award — University Distinguished Alumni Professor, 1980
Western Electric — ASEE Fund Award for Excellence in Teaching and Research (1978)
Sigma Xi Outstanding Young Scientist Award, 1976
Eta Kappa Nu Outstanding Teacher Award, 1974 & 1975

Field of Research Interest

Semiconductor device simulation and modeling, III-V compound semiconductor materials and devices, hot electron transport in semiconductors, ion implantation and radiation damage in semiconductors, thin films and oxides on semiconductors, defects in semiconductors.

Most Recent Refereed Publications (From a total of 119)

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7. K. W. Kim, H. Tian, and M. A. Littlejohn, "Analysis of Delta-Doped and Uniformly-Doped AlGaAs/GaAs HEMTs by Ensemble Monte Carlo Simulations," IEEE Trans. Electron Devices, **ED-38**, 1737, (1991).
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11. M. A. Stroscio, G. J. Iafrate, K. W. Kim, M. A. Littlejohn, H. Goronkin, and G. Maracus, "Transition from Longitudinal-Optical Phonon Scattering to Surface-Optical Scattering in Polar Semiconductor Superlattices," Appl. Phys. Lett., **59**, 1093, (1991).
12. H. Tian, K. W. Kim, and M. A. Littlejohn, "Influence of DX Centers and Surface States on Delta-Doped High Electron Mobility Transistors," J. Appl. Phys., **69**, 4123, (1991).
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Education

08/88   Ph.D. in Electrical Engineering
          University of Illinois, Urbana, Illinois

05/85   M.S. in Electrical Engineering
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02/83   B.S. in Electronics Engineering
          Seoul National University, Seoul, Korea

Work Experience

08/88 - present: Assistant Professor, Department of Electrical and Computer Engineering,
                   North Carolina State University, Raleigh, North Carolina

06/83 - 08/88:   Graduate Research Assistant, Department of Electrical Engineering,
                   University of Illinois, Urbana, Illinois

Academic Honors and Society Memberships

IBM Predoctoral Fellowship (1986-1988)
American Physical Society
Institute of Electrical and Electronics Engineers

Research Interests

Semiconductor physics and modeling of electronic and optoelectronic devices, carrier transport
in bulk and heterostructures, low dimensional effects, quantum transport theory, Monte Carlo
simulation

Selected Refereed Publications (from a total of 54)

K. Kim, B. Mason, and K. Hess, "Inclusion of Collision Broadening in Semiconductor Electron Transport Simulations," *Phys. Rev. B* 36, 6547 (1987).

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